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Zientzia eta Teknologia Fakultateko V. Ikerkuntza Jardunaldiak

V Jornadas de Investigación de la Facultad de Ciencia y Tecnología

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Lankide agurgarriak:

Dakizuen moduan, apirilaren 6an eta 7an Zientzia eta Teknologia Fakultateko V. Ikerkuntza Jardunaldiak izango dira.

Jardunaldiak apirilaren 6an, asteazkena, hasiko dira 8:40ean, hurrengo izenburua duen txostenarekin: **“Una gran Infraestructura de Investigación Europea** (The European Marine Biological Resource Centre) en la **Estación Marina de Plentzia”**, Ibon Cancio irakaslearen eskutik. Jarraian, 9:00etatik 11:30era, esleitutako aretoetan Ahozko Komunikazioak egingo dira aldi berean hainbat arlotarako: I) Biologia; II) Kimika (Kimika Analitikoa eta Kimika Fisikoa), III) Matematika, IV) Ingeniaritza Kimikoa eta V) Geologia. Ahozko Komunikazioak amaitu ondoren, 11:30etik 12:00etara, kafea zerbitzatuko dute eta posterrak ikusteko bisita gidatu bat egingo da Fakultateko Grande Sallean.

Egun horretan bertan, 12:00etan, Paraninfoan V. Jardunaldien Irekiera egingo da, Amaia Esquisabel Eusko Jaurlaritzako Zientzi Politikarako Zuzendariarekin, Carmelo Garitaonandia Bizkaiko Campuseko Errektoreordearekin eta Esther Dominguez Fakultateko Dekanoarekin. Ondoren, María José Sanz Zuzendariak, bc³ Basque Centre for Climate Change-ko Zuzendari Zientifikoak, Hasiera Hitzaldia eskainiko du **“Los retos del Cambio Climático: Un largo camino hasta París”** izenburupean.

[\(Ikusi bideoa\)](#)

Apirilaren 7an, osteguna, emakume ikertzaileei eskainitako saioa izango dugu, Berdintasun Batzordeak sustatua. Txostengile izango dira Nastassja Cipriani Fisika Teorikoa eta Zientziaren Historia Saileko doktorego ikaslea, Leire Ibaibarriaga Aztiko (Tecnalia) ikertzailea eta Itziar Alkorta, Biofisikako Institutuko Zuzendaria.

Saioaren bukaeran “Zientzia eta Teknologia Fakultateko V. Ikerkuntza Jardunaldietako Poster Onenari Saria” emango da. Horren ondoren, kafea zerbitzatuko dute Grande Sallean, eta posterrak ikusteko bisita gidatua egingo da.

Jarraian, 12:00etatik 14:00etara, esleitutako aretoetan Ahozko Komunikazioen bigarren saioa egingo da, hurrengo arloei dagokiena: I) Biologia Molekularra eta Biokimika; eta Bioteknologia, II) Kimika (Kimika Ez-organikoa eta Kimika Organikoa) eta III) Fisika eta Ingeniaritza Elektronikoa.

Jardunaldi hauek gure ikasleentzat oso interesgarriak direnez gero, haien parte-hartzea bultzatzea eskatzen dizuegu, modu horretan ikasgelako presentzialitatea jarduera antolatuetara eramateko.

Zuen laguntza izango dugulakoan, jaso ezazue nire esker on eta agurrik beroena.

Esther Domínguez
Zientzia eta Teknologia Fakultateko Dekano Andrea

Estimados compañeros y compañeras:

Como sabéis, durante los próximos días 6 y 7 de abril se celebrarán las V Jornadas de Investigación de la Facultad de Ciencia y Tecnología.

El miércoles 6 de abril comenzarán las Jornadas a las 8.40 h con la ponencia titulada: **“Una gran Infraestructura de Investigación Europea** (The European Marine Biological Resource Centre) en la **Estación Marina de Plentzia**” impartida por el Profesor Ibon Cancio. A continuación de 9.00 a 11.30 h se presentarán, en las salas asignadas, las Comunicaciones Orales de forma simultánea para las distintas áreas: I) Biología; II) Química (Química Analítica y Química Física), III) Matemáticas, IV) Ingeniería Química y V) Geología. Una vez finalizadas las Comunicaciones Orales, de 11.30 a 12.00 habrá un café y se procederá a una visita guiada a los pósteres, en la Grande Salle de la Facultad.

El mismo día 6 a las 12.00 h se celebrará en el Paraninfo, la Inauguración de las V Jornadas con la presencia de la Directora de Política Científica del Gobierno Vasco, Amaia Esquisabel, del Vicerrector del Campus de Bizkaia, Carmelo Garitaonandia y de la Decana de la Facultad, Esther Domínguez. Seguidamente, tendrá lugar la Conferencia Inaugural a cargo de la Dra. María José Sanz, Directora Científica del bc³, Basque Centre for Climate Change titulada **“Los retos del Cambio Climático: Un largo camino hasta París”**.

[\(Ver vídeo\)](#)

El jueves día 7 de 10.00 a 11.30 h tendrá lugar una sesión dedicada a la mujer investigadora, promovida por la Comisión de Igualdad. Se contará como ponentes con Nastassja Cipriani, estudiante de doctorado en el Departamento de Física Teórica e Historia de la Ciencia, Leire Ibaibarriaga, investigadora en Azti (Tecnalia) e Itziar Alkorta, Directora del Instituto Biofisika.

Al término de la sesión se procederá a la entrega del “Premio al Mejor Póster de las V Jornadas de Investigación de la Facultad de Ciencia y Tecnología”, tras lo cual se servirá un café en la Grande Salle y se procederá a la visita guiada a los pósteres.

A continuación de 12.00 a 14.00 h se presentará, en las salas asignadas, la segunda sesión de Comunicaciones Orales correspondientes a las áreas: I) Biología Molecular y Bioquímica; y Biotecnología, II) Química (Química Inorgánica y Química Orgánica) y III) Física e Ingeniería Electrónica.

Dado que estas Jornadas son de gran interés para nuestro alumnado, os pedimos que impulséis su participación, trasladando la presencialidad del aula a las actividades programadas.

En la confianza de que contaremos con vuestra colaboración, recibid mi agradecimiento y mi saludo más cordial.

Esther Domínguez
Decana de la Facultad de Ciencia y Tecnología

Dear colleagues,

As you know, the 6th and 7th April we will hold the Fifth Conference of Research of the Faculty of Science and Technology.

Wednesday 6th at 8:40 in the Graduate Room the oral presentations of the conference will start with the lecture entitled: **"A big European Research Infrastructure (European Marine Biological Resource Centre) in the Plentzia Marine Station"** given by Dr. Ibon Cancio.

From 9:00 to 11:30 in the assigned rooms, the oral presentations will take place simultaneously for different areas: I) Biology, II) Chemistry (Analytical Chemistry and Physical Chemistry), III) Mathematics, IV) Chemical Engineering and V) Geology. Afterwards from 11.30 to 12.00 there will be coffee and we'll proceed to a guided tour of the posters in the Grande Salle of the Faculty.

That same day at 12:00 in the auditorium the inauguration of the conference will take place attended by the Director of Science Policy of the Basque Government, Amaia Esquisabel, the Vice Rector of Bizkaia Campus, Carmelo Garitaonandia and the Dean of the Faculty Esther Dominguez. After that, at 12.15 is the Inaugural Lecture by Dr. María José Sanz, Scientific Director of the bc³, Basque Centre for Climate Change entitled **"The challenges of climate change: A long way to París"**. ([See video](#))

Thursday 7th from 10.00 to 11.30 in Graduates Room, a session dedicated to **Women in Research** promoted by the Equality Commission will take place. Nastassja Cipriani, Ph.D. student of Theoretical Physics and History of Science Department, Leire Ibaibarriaga, researcher in Azti (Tecnalia) and Itziar Alkorta, Director of Biophysics Institute will participate as lecturers.

After that, the Dean of the Faculty will proceed to give the Award to the Best Poster of the Fifth Conference of Research of the Faculty of Science and Technology. Then, there will be coffee and we'll proceed to a guided tour of the posters in the Grande Salle of the Faculty.

That same day from 12.00 to 14.00 in the assigned rooms, the rest of oral presentations will be presented simultaneously for different areas: I) Molecular Biology and Biochemistry II) Chemistry (Inorganic Chemistry and Organic Chemistry) and III) Physics and Electronic Engineering.

As you can see, these conferences are of great interest to students.

Therefore, we ask you to promote participation, transferring classroom presence to the activities scheduled.

Best regards,

Esther Domínguez
The dean of the Faculty of Science and Technology



A big European Research Infrastructure (European Marine Biological Resource Centre) in the Plentzia Marine Station

Ibon Cancio

CBET Research Group. Dept. of Zoology and Animal Cell Biology, Faculty of Science and Technology. Research Centre for Experimental Marine Biology and Biotechnology (PiE-UPV/EHU). Areatza w/n. E48620. Plentzia.

KEY WORDS: ESFRI roadmap, EMBRC, Research Infrastructures, marine biological resources, marine biotechnology

In the year 2006 the European Commission launched its first roadmap of European Research Infrastructures (ESFRI roadmap), for the update of already existing RIs and the implementation of those considered necessary to boost the research and technology transfer capacities of European countries. The European Marine Biological Resource Centre, EMBRC (www.embrc.eu), is a disseminated RI formed mainly by marine biological stations belonging to Universities, which is placed in the ESFRI roadmap since 2008. During its preparatory phase, funded by the European FF7 and H2020 programs, EMBRC has been endorsed by 9 different countries (Belgium, France, Greece, Israel, Italy, Norway, Portugal, Spain, UK). The Plentzia Marine Station (PiE-UPV/EHU) was invited to join in 2013, and together with the Marine Station of the University of Vigo (ECIMAT) constitutes the Spanish node of EMBRC in representation of Spain, as approved and signed by the Spanish Ministry of Economy and Competitiveness (MINECO) in September 2014. Recently, the Rectors of both Universities officially signed the collaboration agreement towards formalising the formation of such Spanish node.

The mission of EMBRC is to foster the full development of Marine Biotechnologies and provide advanced research capabilities for the valorisation of marine biological resources in Europe, as envisaged in the European Blue-Growth strategy. EMBRC activities will be focused around the:

- Organisation and funding of access (to academia and private sector) to its installations and services;
- Joint development of key enabling technologies (in collaboration with users);
- Knowledge & technology transfer to industry and policy makers;
- Training & education in marine biological sciences & technology;
- Legal clearance for access to marine biodiversity (Nagoya protocol);
- Construction of an e-infrastructure, collaboration and interoperability with other RIs.

The distributed nature of EMBRC allows access to most of the marine ecosystems and their biodiversity in European littoral waters and the Red Sea, providing know how in the implementation of modern molecular biology and advanced microscopical analysis of such biota. Access to these resources could be provided remotely, this including database and collections, or on site. Access will be granted through service level agreements that will be managed centrally from the headquarters established in the University Pierre and Marie Curie in Paris.

The legal structure selected to operate EMBRC is an ERIC (European Research Infrastructure Consortium) that was created by the European Union for the functioning of disseminated research infrastructures. During 2015 and 2016 the EMBRC implementation board, with a scientific representative of PiE-UPV/EHU has been elaborating the budget, business plan and statutes of EMBRC-ERIC that were presented, 1st Step, by the French Government for evaluation by the European Commission in April 2016. Upon approval in June 2016 of these statutes, 2nd step application is envisaged for late 2016, so EMBRC-ERIC could become fully operative in 2017. In the meantime EMBRC has applied for H2020 infrastructure research projects with a high rate of success.

From its participation in EMBRC, PiE-UPV/EHU and the University in general will obtain the following benefits:

- Networking possibilities at European/world level.
- Scientific collaborations, exchange of researchers, technologies and know-how.
- New research strategic objectives and diversification of research lines.
- Local social and international visibility.
- Connection to industry and market.

ACKNOWLEDGEMENTS: Participation of PiE-UPV/EHU in EMBRC is made possible thanks to the financial support of Diputación Foral de Bizkaia (PiE EMBRC DFB15/01), UPV-EHU and European Commission (H2020-INFRADEV-2-201515/01).

BIOZIENTZIAK: INGURUNE ALDERDIAK

BIOCIENCIAS: ASPECTOS AMBIENTALES



Forensic entomology in the Basque Country.

Actual situation

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UPV/EHU

KEY WORDS: Insects, Calliphoridae, distribution, biology, forensics, molecular, protocol, entomotoxicology

Forensic Entomology applies the knowledge developed about the structure and dynamics of insect and other arthropod communities as evidence in criminal (and civil) cases, as they must be solved by the Court of Justice. Although it is a discipline not yet adequately developed in our country, its knowledge can be traced back to the thirteenth century thanks to the reports recorded by a magistrate that have recently been translated into English under the title "Collected Cases of Injustice Rectified or The washing away of wrongs". In the book are described cases solved by the prefect Sung Tz'u or Sòng Cí (1186-1249), a medical doctor who managed to incriminate a murderer thanks to the presence of flies deposited on the sickle with which the victim was killed, although the weapon had been cleaned by the murderer. The attraction of flies to blood and other animal remains is well known. In fact, it was used by the Italian naturalist physician Francesco Redi (1626-1697) in 1668 to displace the presumption of spontaneous generation thanks to his experiment as he was trying to understand the origin of the "worms" developed on animal remains. Such worms did not result from the transformation of rotten flesh, they born from eggs previously deposited by carrion flies on the remains. Thus, the latin term corpse (cadaver) refers to these "worms" (fly larvae) that are used in the dating of the meat: Flesh, Date, Worm (Caro, Data, Vermes). Taking into account that the development of insects depends on the ambient temperature, an adequate knowledge of the environmental conditions together with the correct identification of the pioneer species that colonises a body allow us to establish precisely when this first insect arrived, colonized this corpse and, thus, we can estimate the date of death also known as postmortem interval (PMI) based on the period of insect activity (PIA).

Based on these premises, one of the first objectives of our research group was the knowledge of the species of Calliphoridae (blowflies), as colonizers of corpses, in the Autonomous Community of the Basque Country (CAPV), the periods when adults (flies) are active, and their development patterns under controlled conditions. Moreover, we analyse alterations in its cycle due to the presence of parasitoids or the ingestion of toxicants. Finally, a sample of each species has been molecularly characterized to facilitate the species identification in degraded samples or preimaginal instars when breeding is not possible and we have no adults for the correct identification of the species based on morphological characters.

The work has allowed us to establish the first reference collection of necrophagous insects of forensic interest in the Basque Country, opening new and pioneer research topics in Spain.

Finally, we have adequated the protocol of actuation and collection of samples of entomological origin in the Basque Country during a crime scene inspection, revised and updated, incorporating the recognition, collection and conservation of mites associated to cadaveric remains, and proposed the first mite as forensic indicator (*Proctolaelaps euserratus* Karg, 1994). This protocol has been published in Basque and Spanish (bilingual) to facilitate the incorporation of entomological evidence during criminal and civil investigations in the Basque Autonomous Community.

Analysis of food quality of litter for epigeic earthworms: *Eisenia andrei* as a case study

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KEY WORDS: *Eisenia andrei*, Growth, Survival, Grass, Pre-composted, Organic matter

Epigeic earthworms are considered ecosystems engineers since they modify organic matter cycles and properties on soil. Claimed as natural fertilizers, they produce casts with nutrients easily assimilable by plants. For this reason, in sustainable agriculture fertilization of soil should be linked to the maintenance and enhancement of earthworm activity. Grass remnants from grass cutting practices are usually left composting in the open air contributing to formation of new soil layers via decomposition by soil organisms. In this context, our objective has been to test the suitability of grass to support active populations of the earthworm *Eisenia andrei* focused on the earliest stages of the vital cycle. We evaluated eclosion success, survival and growth of new born animals individually incubated under constant temperature and humidity regime in grass composted for 1 to 13 weeks. Biochemical analysis of substrates revealed increasing mineralization and decreasing fibre percentage associated to composting period. Protein content increased in the first 7 weeks decaying in the latest period of grass evolution while lipid and soluble carbohydrates remained constant. A decay in eclosion success associated to aging was found (from 60% after 1 week to 40% after 13 weeks) and survival percentage decreased linearly with mineralization according to the equation: $\text{Survival \%} = 120.03 - 1.4085 \times \text{Inorganic matter \%}$. Growth patterns for newly hatched *Eisenia andrei* differed largely between grass substrates and we obtained average maximal live weights (MLW) of 119, 107, 64, 57 and 70 mg in pre-composted grass for 1,3,7,11, and 13 weeks respectively. These patterns are related to organic content, being the fibre component the key factor to understand the physiological responses. Grass aging reduces the labile components of fibre decreasing biochemical quality of nutrients accessible to young earthworms (i.e higher digestive costs) redounding in lower life expectancies and growth.

Genetic analysis of Spondyloarthropathies: an evolutionary approach

Imanol Martín¹, Montserrat Hervella¹ Neskuts Izaguirre¹ and Concepción de la Rúa¹
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KEY WORDS: Spondyloarthropathies, genes, *HLA-B27* allele.

The Spondyloarthropathies (SpA) is a group of rheumatic diseases in which the immune system is implicated, involving inflammation, deformation and sometimes fusion of the different joints. These changes reduce considerably a patient's life quality. Although the accurate etiology of SpA is unknown, the disease's development has demonstrated to be influenced by a combination of genetic and environmental factors. However, polymorphisms within different genes associated with the development of these diseases have been discovered. In this study, 43 individuals showing different SpA, were analyzed from the medieval burial site of San Miguel de Ereñozar (Ereño, Bizkaia). The aim of this study is to relate these pathological phenotypes with different genetic variants according to GWAS studies (Genome-Wide Association Study). Nuclear markers (*HLA-B27* allele, *IL-23R* and *ERAP1* genes) associated with were analysed in the different burials, and *HLA-B27* allele, the most significant genetic marker associated with ankylosing spondylitis, was found in several individuals. Once described the different mutations of these pathologies and given the lack of clear differential diagnostic criteria for early stages of SpA, the determination of an haplotype associated with these diseases will contribute to the early diagnosis of SpA in the current population.

ACKNOWLEDGEMENTS: This work is possible thanks to funds the Basque Government (IT542-10, PRE_2014_1_326). UPV-EHU (UF111/09) and the Spanish Ministry of Science and Innovation (GCL2011-29057/BOS).

NANOSILVEROMICS: Uncovering the mechanisms of toxic action of silver nanoparticles in model alternative aquatic and terrestrial organisms

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KEY WORDS: Ag NPs, nanotoxicology, aquatic and terrestrial organisms.

Manufactured nanoparticles (NPs) are already being incorporated in many consumer products, with domestic, medical, cosmetic and industrial uses. Concomitantly with the increasing applications of nanosized materials, concerns are growing because the novel properties of nanostructured materials and their potential input in ecosystems could lead to unknown health or environmental hazards. Silver NPs (Ag NPs) are the most widely used metal NPs due to their unique optical and catalytical properties and efficient antimicrobial activity. Previous studies have reported that NPs may enter aquatic systems directly through aerial deposition, effluents, dumping and run-offs. Predictions estimate that between 0.07 ng/L and 40 µg/L of Ag NPs released from consumer products will be found in the aquatic environment. In the terrestrial environment, the major source of NPs deposition is through the disposal of wastewater treatment plants (WWTP) biosolids, mainly after their land application, and is estimated that Ag NPs concentration in soils with biosolids in Europe ranges from 1.33 to 4.44 mg/kg. Once in the environment, Ag NPs can interact in different ways with living organisms, including mussels and fishes in aquatic environment and earthworms in the terrestrial compartment. Therefore, for an integrated approach, three model organisms were employed: 1) marine mussels *Mytilus galloprovincialis*, filter-feeding bivalves which are important targets of nanomaterials entering the water column and suitable sentinels to monitor NP impact into the marine environment, 2) freshwater zebrafish *Danio rerio*, a consolidated experimental model in biomedicine, at embryo and juvenile-adult developmental stages, and 3) earthworms *Eisenia fetida*, terrestrial model organisms widely used as bioindicators of soil pollution and as test organisms in standard toxicity tests. Toxic effects of Ag NPs have been studied generally at concentrations orders of magnitude higher than those expected in the environment, whereas in this work experiments included environmentally relevant Ag NP concentrations. Mussels and zebrafish were exposed to Ag NPs through water and diet (algae *Isochrysis galbana* and the crustacean *Artemia sp.*, respectively), whereas earthworms were exposed through artificially contaminated soils.

In the present study, ICP-MS and autometallography demonstrated Ag accumulation mainly in digestive organs of the three species, which indicated that animals were taking Ag NPs especially through the diet. In mussels, Ag accumulation was higher during the resting period than in the reproductive stage and season-dependent changes were also evidenced in the biological responses measured. Ag NP exposure elicited changes in gene and protein expression profiles and responses at cellular and tissue levels, including lysosomal membrane destabilization and genotoxicity, even at environmentally relevant concentrations, in the three model species. Main mechanisms of action of Ag NPs involved oxidative stress, DNA damage, alterations in the membrane transport functions and disruption of actin cytoskeleton whereas lysosomal activation and stimulation of phagocytosis could represent defensive responses. As to higher level effects, water-borne exposure of zebrafish to environmentally relevant Ag NPs concentration (100 ng/L) caused significant impairment in zebrafish reproduction (reduction in the number of spawned and viable eggs). Similarly, embryo development was impaired after parental exposure of mussels to 1 µg/L Ag NP concentration and a severe reduction in the number of juveniles and cocoons was recorded in earthworms ($EC_{50\text{reproduction}}=17.92$ mg Ag NPs/kg), suggesting a severe affection in the reproductive output. Overall, the results obtained in the Nanosilveromics project have greatly contributed with knowledge on the mechanisms of action and toxicity of Ag NPs and suppose a step forward in environmental risk assessment of Ag NPs in both aquatic and terrestrial environments. Funded by: Univ. Basque Country (UFI 11/37, PhD fellowships), Basque Government (Cons. Res. Groups; IT810-13), Spanish MINECO (Nanosilveromics Project) and EU COST ES1205 (ENTER). Technical and human support provided by SGiker (UPV/EHU, MICINN, GV/EJ, ESF) is gratefully acknowledged.

Crop adaptation to climate change

Jon Miranda-Apodaca¹, Ander Yoldi-Achalandabaso¹, Arantza del Canto², Maite Lacuesta², Amaia Mena-Petite¹, Usue Pérez-López¹ and Alberto Muñoz-Rueda¹

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KEY WORDS: barley, climate change, drought, elevated CO₂, grassland, high temperature, plant physiology, salinity.

The atmospheric CO₂ concentration has increased since the beginning of the industrial revolution, from a concentration of 280 µmol mol⁻¹ to the current concentration of 400 µmol mol⁻¹, mainly due to anthropogenic causes, such as consumption of fossil fuels (coal, oil and natural gas) and changes in land use such as agriculture and rapid deforestation. Besides increasing the concentration of CO₂, rainfall patterns are expected to change, increasing extreme events of drought and flooding due to the change in the distribution of rainfall. These global climatic changes can have major consequences for the terrestrial vegetation, such as short-term physiological responses in crop plants and long-term changes in the structure and function of ecosystems, affecting, ultimately, the productivity of plant communities. Additionally, due to the increase in human population, an increase in food production is needed to sustain the growing human population.

We investigated the effect of climate change on barley growth under drought and salt conditions. Both water stresses reduced plant growth, however, in both cases, the elevated CO₂ mitigated the negative impact of the water stress, although the mechanism was different. On one hand, under drought conditions, the plant achieved higher growth due to stomatal adjustment and, on the other hand, under salt conditions, the plant showed higher growth thanks to a higher osmotic adjustment.

We also analyzed the impact of climate change on grassland communities. The high CO₂ and drought had antagonistic effects and differences between functional groups were observed, and these effects also varied depending on the type of competition. Under future climatic conditions, in mixture, the legumes will be favored at the expense of the grasses.

In all the studies, when the plants were subjected to a water stress, the plants tended to increase their concentration of antioxidants as a defense mechanism. In order to try to take advantage of this fact, we performed an applied research using lettuce under salinity, high light, and elevated CO₂ conditions. We used short periods of stress and we were able to increase the quality of the lettuce without losing its yield.

Looking to the future, we want to continue our experiments on basic and applied research regarding to climate change -high temperature, drought, and elevated CO₂ alone or in combination- and its consequences on food and feed production and quality.

Ecosystem Services Assessment of the Basque Country: Bridge between science and management

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KEY WORDS: Biodiversity, Ecosystem Services, science-policy interface.

Ecosystem Service Framework provides a space for coordination and dialogue between scientist, managers, politicians, NGO representatives and other stakeholders. The Ecosystem Services Assessment of the Basque Country develops an approach of integrative knowledge that enhances the link between science, policy-making and society. Due to its applicability for management, the perspective of ecosystem services can contribute to develop sound land-use sustainable policies and planning actions at different scales.

The principal research lines carried out in the Basque Ecosystem Services Assessment to promote the implementation of sustainable biodiversity and ecosystem services management policies are:

1. Ecosystem services evaluation using biophysical, social and economic indicators.
2. Mapping ecosystems services at different scales.
3. Analyzing social preferences (demand) and users' perceptions through participatory processes (e.g. face to face interviews, stakeholder workshops).
4. Developing future scenarios: qualitative (participatory) and quantitative (modelling).

In all these research lines scientist collaboratively work with politicians and specialized technicians of the local and regional administration to favour the real implementation of the research results into landscape management.

Relevant policy implementations of the results of this broad research are already taking place in the Basque Country. Examples include:

- The Urdaibai Biosphere Reserve Master Plan for Use and Management (MPUM) includes the protection of the mixed oak forests thanks to the results of our assessment.
- The Bilbao Metropolitan Landscape Planning (PTP) and The Regional Planning Guidelines for the Basque Country (DOT) are going to include the ecosystem services maps generated in the assessment.
- Ecosystem services indicators are likely to be included in Basque official statistics.

According to our experience, the inclusion of applied science in decision making processes favours adaptive and resilient landscape management.

Vibrio spp. in the coastal waters of Bizkaia

E. Ogayar¹, M. Orruño¹, V.R. Kaberdin^{1,2} and I. Arana¹

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²IKERBASQUE, Basque Foundation for Science.

KEY WORDS: *Vibrio*, distribution, identification.

Members of the *Vibrio* genus are ubiquitously present in marine ecosystems. Although their life cycles and viability can be influenced by the fluctuation of temperature, salinity and availability of nutrients, temperature is believed to be the main factor that controls *Vibrio* survival in the marine environment. This assumption is consistent with the seasonal distribution of culturable *Vibrio* in coastal environments. Thus, a reversible reduction in the number of culturable vibrios during the winter season followed by their increase in the summer time has been described.

The global warming inevitably leads to an increase in the temperature of surface waters and is likely responsible for the recent outbreaks of *Vibrio*-associated diseases in European countries. In this context, it is noticeable the lack of data concerning the seasonal distribution of *Vibrio* species in the coastal water of the Basque Country, especially if we consider the ecological, economic and tourist importance of coastal areas of our territory.

The aim of our work was to quantify and identify the *Vibrio* species present in the coastal water collected from three different areas (Astondo, Armintza and Laida) in the Bay of Biscay. To determine the distribution and abundance of *Vibrio* populations, seawater samples from sampling stations were collected along a year and total bacteria, heterotrophic culturable bacteria (on Marine Agar) and presumptive culturable *Vibrio* (on TCBS and CPC media) were determined. The results showed a seasonal distribution of culturable bacteria, including *Vibrio*, with a higher presence during the warm season reaching $2.2\text{--}4.4 \times 10^4/\text{ml}$ and $1\text{--}3 \times 10^2/\text{ml}$, respectively.

161 of the *Vibrio* likely colonies grown on TCBS or CPC agar were biochemically identified by using API 20E test (Biomerieux), and only the 29.2% of them were classified as *Vibrio* species. This fact indicates that TCBS and CPC media, recommended for the selective isolation and culture of *Vibrio* spp. from clinical specimens, are not appropriate to isolate *Vibrio* spp. from natural seawater samples.

Identified *Vibrio* species were further verified by 16S RNA gene sequencing. The final identification of some isolates was achieved on the basis of multilocus sequence analysis (MLSA) by using the housekeeping genes: *gapA*, *ftsZ*, *topA*, *mreB*, *gyrB*, *pyrH* and *recA*. We found that most of the identified *Vibrio* belonged to the *Splendidus* and *Orientalis* clusters.

Survival strategies of *Vibrio harveyi* and *Escherichia coli*

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KEY WORDS: *Vibrio*, *Escherichia*, survival strategies

In their natural ecosystems, bacteria are continuously exposed to changing environmental factors including physicochemical parameters (e.g. temperature, pH, etc.), availability of nutrients as well as interactions with other organisms. To confer resistance to these stresses and increase their survival under adverse conditions, bacteria trigger a number of adaptation mechanisms.

We have studied the survival strategies developed by two model strains, *Vibrio harveyi* and *Escherichia coli*, exposed to adverse physicochemical factors. *V. harveyi* is a marine bacterium, adapted to saline environments where it is exposed to nutrient scarcity and temperatures below its optimum for growth. In contrast, *E. coli* is a copiotrophic bacterium commonly found in the intestines of warm-blooded organisms and, therefore, it is an allochthonous bacterium in natural aquatic systems.

Along survival experiments carried out under laboratory conditions that mimic environmental situations (starvation/famine, suboptimal temperatures, luminous irradiation, etc.), we have determined the morphological and physiological changes of both bacteria and established the survival strategies that they develop to cope with adverse conditions. Our results indicate that these bacteria are able to adopt the viable but nonculturable (VBNC) phenotype. This phenotype corresponds to the physiological state of cells that become nonculturable but retain their metabolic activity. Under these survival conditions, we have also determined their ability to develop the *bust and boom* strategy. In this last survival model, most cells die upon stress, and the few survivors subsist at the expense of the dead cells.

We have found differences between these bacteria in the conditions inducing the VBNC state, in the capacity to recover culturability after reversion of adverse conditions, as well as in the biological significance of the VBNC state. Thus, *V. harveyi* enters into the VBNC state by effect of short exposure to low temperature (4°C) or visible light or after a long maintenance at 20°C. Moreover, under appropriate environmental conditions, VBNC and culturable *V. harveyi* subpopulations are able to resuscitate and to regrowth, respectively. So, VBNC and *bust and boom* strategies ensure the success of *V. harveyi* populations in the environment.

E. coli adopts the VBNC phenotype at 20°C by effect of nutrient scarcity or visible radiation. For this bacterium, the exposure to low temperature (4°C) only decreases metabolism to assure the permanence of total population. Moreover, VBNC *E. coli* cells are not able to resuscitate under tested conditions. For this bacterium, the formation of VBNC cells is destined to provide nutrients for the maintenance of the culturable fraction, and general survival strategy seems to correspond to the *boom and bust* strategy.

Study of the effect of a monoclonal antibody against *Candida albicans* mannoprotein

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KEY WORDS: *Candida albicans*, Immunocompromised, Cancer, Mannoproteins, Kre9.

Candida albicans is a dimorphic fungus that can grow in both yeast and filamentous forms. It is a commensal microorganism, but it can disseminate through the blood when the patient is immunocompromised, causing an invasive candidiasis. Once in the blood, the liver is the main organ responsible for the clearance of the infection. In this organ, yeasts adhere to endothelial cells of blood vessels, leading to an inflammatory process. This process recruits immune cells through expression of cytokines and adhesion molecules in order to clear the infection. Our research group hypothesized that since oncological patients are commonly immunosuppressed mainly due to chemotherapy treatment, the inflammatory response could make possible that tumour cells present in the blood adhere to the liver endothelium instead of immune cells. This may lead to the formation of a metastatic focus in the liver.

As IL-1B cytokine is one of the most important involved in inflammatory processes, an anti-IL-1B antibody was used to detect putative cross-reactivities with *C. albicans* and, in this way, the mannoprotein Kre9 was identified. This work is focused on the study of the effect of a monoclonal antibody developed against this mannoprotein.

To obtain the monoclonal antibody, we first produced the recombinant Kre9 in an *Escherichia coli* model, and then, the protein was used to produce the antibody in mice. Thirteen antibodies were obtained, and the most reactive one was chosen for the experiments. On the one hand, the effect of the antibody over the adhesion of tumour cells to mice endothelial cells was tested. On the other hand, the effect over the yeast was assessed, by testing the growth and germination, a critical virulence factor, of the yeast in presence of the antibody. Finally, the ability of the antibody to recognize the fungus through an Indirect Immunofluorescence (IIF) was explored. In the experiments conducted to test the effect of the antibody over the yeast, 6 different strains of *C. albicans* were used; a reference strain, two isolates of invasive infections and three isolates of oral candidiasis. It was found that the antibody was able to reduce the adhesion of tumour cells to endothelial cells. Unfortunately, no growth reduction was seen in growth curves, and, surprisingly, the highest concentration tested, 1 µg/ml, induced the growth of the yeast. When incubated 18 h in PBS, only one strain showed reduction in yeast numbers and an induction of the growth was again observed at the highest concentration of the antibody tested. However, the germination of *C. albicans* was reduced in all the strains about a 13%. In the case of the IIF, the antibody was also successful in recognizing only the hyphae of the fungus and not the yeasts. Moreover, the hyphae of *C. dubliniensis*, the only other species from *Candida* genus able to form true hyphae, were not recognized by the anti-Kre9 antibody. We are currently studying the ability of the antibody to reduce the growth of the fungus in presence of antifungal drugs, and its ability to reduce biofilm formation, which is related to the hyphae formation. Finally, in case that promising results are obtained, we will proceed to test the effect of the antibody in an *in vivo* murine model.

In conclusion, the developed antibody could be useful for the differentiation between the yeast and hyphae of this fungus, and between *C. albicans* and *C. dubliniensis* infections. These results prove that the study of the mannoproteins of *C. albicans* could lead to the discovery of new therapeutic and/or diagnostic targets.

AA and IB are recipients of a predoctoral grant from the Basque Government and AP has been recipient of a predoctoral grant from the UPV/EHU.

Study of *Lomentospora prolificans* pathogenicity: Host immune response and fungal virulence factors

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KEY WORDS: Proteomics, immunomics, antifungal resistance, host-pathogen interactions.

The filamentous fungus *Lomentospora prolificans* is an opportunistic pathogen whose prevalence in clinical settings has increased in the last decades. Moreover, *L. prolificans* is inherently resistant to all the antifungal compounds available nowadays. As an opportunist, *L. prolificans* mainly infects patients suffering from underlying conditions, most of them related to immunosuppressed states (transplant recipients, AIDS patients, etc.). In addition, this species is prone to get disseminated through the bloodstream, being this the most usual pattern of infection and the one associated with the highest mortality rates. In order to deeply understand *L. prolificans* pathogenesis, we are performing a multifaceted analysis of fungal virulence factors and host immune responses to this species by applying molecular and cellular approaches, with the final goal of finding novel candidates for developing therapeutic or diagnostic tools.

Decoding the humoral recognition of *L. prolificans* by immunoproteomics

Protective antifungal antibodies may play important roles during fungal infections, especially in the absence of a proper innate immune response. Identification of key antigens is crucial as they could represent potential targets for passive immunotherapy. In this sense, we have identified a wide range of antigenic proteins reactive with IgA and IgG from immunocompetent individuals by using immunoproteomics-based techniques, coupled with LC-MS/MS. Interestingly, Heat shock protein (Hsp) 70 was found to be recognized by the two Ig isotypes, and in the two fungal morphotypes, conidia and hyphae. This fact proves the high immunogenic properties of Hsp70, making this protein very interesting for the development of therapeutic strategies.

Uncovering antifungal resistance mechanisms

As previously mentioned, *L. prolificans* presents an inherent resistance to conventional antifungal drugs. This makes it difficult to successfully treat these infections, increasing mortality rates. However, in-depth analysis of the molecular basis of this resistance could be a key in the development of new drugs or therapeutic strategies. Therefore, we are analyzing proteomic, morphological and structural changes in fungal cells in the presence of voriconazole, which is the antifungal drug that has shown the best results against *L. prolificans*. Interestingly, the microbe is able to alter its cell wall architecture and carbohydrate composition after being exposed to the drug, also modifying the abundance of some cell wall-associated proteins. Among others, we detected the chaperone Hsp70, which seems to be involved in triggering protective signaling pathways in response to different stresses, including the presence of antifungal drugs.

Future perspectives

Given the importance that Hsp70 seems to have, in the near future our research group will focus on determining the exact role that this protein plays in key processes such as fungal virulence, induction of host immune response, and antifungal resistance. To do that, we are constructing knockout strains for this protein and testing several Hsp70-specific inhibitors to analyze their potential as novel therapies.

This work is supported by a General Grant to Consolidated Research Groups UPV/EHU 2011-2014, UFIMEMPVES (UFI11/25) and EHUA13/14 projects from the UPV/EHU. AP, AA and IB are recipients of FPI grants from the UPV/EHU and the Basque Government.

Transcriptomic study of *Aspergillus fumigatus* during a murine intranasal infection

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KEY WORDS: *Aspergillus fumigatus*, Intranasal infection, Microarray.

BACKGROUND

Aspergillus fumigatus is the most ubiquitous airborne pathogenic mold worldwide, capable to produce high mortality rate in immunodeficient patients. In this kind of patients the fungal is able to avoid the weak macrophage response and finally penetrates the alveolar epithelium and germinate creating invasive hyphae that are able to disseminate through the bloodstream causing fungal disseminated diseases, named invasive aspergilosis (IA). Nowadays, to deepen into the biology of this fungus and improve therapeutic and diagnostic methods, fungal virulence factors are studied using animal infection models and transcriptomic technologies. Therefore, our research group performed an intranasal infection model, in order to study the fungal behavior using a customized microarray expression.

METHODS

Three independent intranasal experimental infections of immunosuppressed mice with 10^7 *A. fumigatus* conidia resuspended in saline solution were carried out. Two daily animals were sacrificed and their lungs were extracted during the following 4 days in order to obtain total RNA for studying the transcriptomic fungal profiles during the first steps of a lung infection, using the AWAFUGE v.1 microarray designed by our research group. The results were validated by RT-qPCR using 48 genes chosen after data analysis using a modified R code based on Bioconductor and limma libraries.

RESULTS

After analyzing the microarray results, around 1% of the *A. fumigatus* genome (108 genes) was differentially expressed during the process relative to the first day of the infection. 93 of them were down-regulated genes while 15 of them were up-regulated during the process. Among the down-regulated genes, 12 of them are implicated in 25 metabolic pathways, where it is noteworthy to highlight tryptophan metabolic pathway and CTA cycle pathway. Furthermore, among these genes there are five of the principal *A. fumigatus* secreted proteins described in the literature (Asp f1, Mep/Asp f5, DppIV, DppV y ChiB1). In contrast, there is no virulence related genes among the up-regulated during the process. Finally, the results were validated by RT-qPCR obtaining a Pearson's R value of 0.88.

CONCLUSIONS

- 108 genes presented a differential expression pattern during the infection process.
- Secreted proteases are weapons used by the mold to progress in the lung tissue to produce an infection.
- *A. fumigatus* virulence response seems to start before in the first 24 hours after infection.
- 25 metabolic pathways are differentially expressed, at least in one of their reactions during the progress of infection.

Biological synthesis of magnetic nanoparticles

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KEY WORDS: magnetotactic bacteria, magnetosomes, extraction and purification.

Magnetic nanoparticles are subject of intensive research due to their interesting properties applicable to fields such as biomedicine or biotechnology. In particular, iron oxide nanoparticles, like magnetite or maghemite nanoparticles, have attracted great attention because of their biocompatibility and high oxidative stability, being the optimal candidates for Magnetic Resonance Imaging (MRI), drug delivery or magnetic hyperthermia based cancer treatment. The synthesis and final characterization of these nanoparticles determine their latter use, and parameters as shape, size distribution and chemical quality have to be controlled carefully in order to produce the desired characteristics.

Currently there are several chemical synthesis methods to produce magnetite nanoparticles. Even though chemical syntheses are the main widespread techniques used because of their high yield and quickness, they present some disadvantages such as low degree of crystallinity and large polydispersity. In order to avoid these outcomes, an alternative method is proposed: biological synthesis by magnetotactic bacteria.

Magnetotactic bacteria are defined as motile aquatic prokaryotes with the ability to swim along the Earth's geomagnetic field lines due to the presence of intracellular structures called magnetosomes. Magnetosomes are magnetic nanoparticles composed of a mineral core of magnetite or greigite surrounded by a lipid bilayer membrane (1). These biogenic nanoparticles show a huge variety of shapes and sizes -ranging from 40 to 120 nm- and it is dependent on bacterial species. According to current theory, magnetotactic bacteria would produce these organelle-like nanostructures in order to locate and maintain an optimal position in chemical and redox gradients along the water column (2).

In this work, we explore the biological synthesis of magnetic nanoparticles by the extraction and purification of magnetosomes from cultures of *Magnetospirillum gryphiswaldense*. Furthermore, we optimize the extraction process by comparing two mechanic cell lysis procedures (*French Press* and *Cell Disruptor*, applying three different pressures). Three main techniques are used to check the quality of the isolated magnetosomes: *Vibrating Sample Magnetometer* (VSM) for the magnetite quantification and *Transmission Electron Microscopy* (TEM) and *Fourier Transform Infrared Spectroscopy* (FT-IR) for the structural characterization of the nanoparticles. In addition, we measure the aggregation behaviour of magnetosomes and stability in aqueous solution by means of *Dynamic Light Scattering* (DLS).

We consider the cell lysis a crucial step that determines hugely the efficacy of the extraction process. The *French Press* at 20 ksi seemed to be the best method for magnetosome extraction based on the amount and quality of the magnetosomes obtained. The magnetosomes were structurally characterized as cuboctahedral particles with an average diameter of 45(±3) nm (3). TEM images showed a limited presence of cell debris that was identified as poly-**B**-hydroxybutyrate (PHB) by FT-IR. The Zeta potential of the magnetosomes suspended in water was always lower than -30mV, which indicates a moderately stability.

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BIOZIENTZIAK:
ALDERDI MOLEKULARRAK

BIOCIENCIAS:
ASPECTOS MOLECULARES



Metalloproteinases 2 and 9 mediate the chemotactic effect of ceramide 1-phosphate in macrophages.

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KEY WORDS: Chemotaxis, metalloproteinases, sphingolipids.

The bioactive sphingolipid ceramide 1-phosphate (C1P) is implicated in inflammatory responses and was recently shown to promote cell migration. However, the mechanisms involved in these actions are poorly described. Here we show that C1P stimulates the activity of the matrix metalloproteinases 2 and 9 (MMP-2 and MMP-9) in J774A.1 macrophages. When looking into the mechanisms involved in this process we observed that C1P potently stimulated the phosphatidylinositol 3-kinase (PI3K)/Akt and mitogen-activated protein kinase (MEK)/extracellularly regulated kinases (ERK) pathways in the macrophages, suggesting a possible involvement of these pathways in the activation of MMP-2 and MMP-9. Noteworthy, inhibition of these kinases with specific siRNA blocked C1P-stimulated MMP-2 and MMP-9 activity. Of importance, pharmacological inhibition of MMP-2 and MMP-9 with selective inhibitors or treatment with specific siRNA to silence the genes encoding these kinases potently decreased C1P-stimulated cell migration. Hence, it can be concluded that C1P promotes cell migration through stimulation of MMP-2 and MMP-9 activation. Moreover, we demonstrate in this work that activation of these MMPs and C1P-stimulated cell migration can be blocked by pertussis toxin, suggesting the intervention of a G_i protein-coupled receptor in these actions.

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Genetic Risk Factors for Injuries in Football

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KEY WORDS: genetics, injuries, football.

EXERCISE-RELATED INJURIES CAN HAVE A NEGATIVE IMPACT ON QUALITY OF LIFE

Exercise has great health benefits, but it also increases the risk of suffering musculoskeletal injuries. Injuries might have negative short- and long-term health consequences that could reduce quality of life. Therefore, individualized injury prevention programmes need to be implemented in order to take full advantage of exercise and promote healthy ageing. To do so, it is necessary to investigate risk factors and develop screening tools to identify those at risk.

GENETIC VARIANTS AND THE RISK OF MUSCULOSKELETAL INJURIES

Investigating the contribution of genetic variables to the risk of injury offers great potential. Several single nucleotide polymorphisms (SNPs) have been associated with anterior cruciate ligament rupture and chronic Achilles tendinopathy using a candidate gene approach. These SNPs are located in genes encoding the components of connective tissue, namely, collagens, proteoglycans, glycoproteins and elastin; or the proteins involved in their regulation and maintenance. However, the number of studies is small, replication of the results is lacking and the candidate gene approach is limiting. Thus, the aim of the following two research projects is to further investigate the association between genetic variants and the risk of injury in elite football players.

CURRENT PROJECTS IN THE SPORT GENOMICS RESEARCH GROUP

1. In collaboration with Athletic Club and BAIGENE, the association of injuries with 170 previously investigated SNPs and other physical and medical variables is being investigated in 135 elite football players. Genetic and non-genetic variables will be integrated in a multifactorial model aimed at identifying those at high risk of suffering specific injuries. In particular, little is known about the influence of common genetic variants on the risk of sustaining muscle injuries, which are the most frequent injuries in football. Hence, the present project will provide novel insights on this topic; albeit on a small sample size and using a candidate gene approach, which are important limitations.
2. To overcome the aforementioned limitations, a second project is under preparation where a large number of elite football teams from Europe are currently being recruited. Teams will prospectively send player data and injury reports, and their association with thousands to millions of genetic markers will be investigated using whole-genome screening methods.

These studies will hopefully shed light on the contribution of genes to the risk of exercise-related injuries and advance the development of screening tools necessary to promote safe exercise participation.

Development of a PCR-based methodology for Gene Doping detection

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KEY WORDS: Sports, Gene Doping, Detection.

The illicit use of drugs has always been a common practice among athletes in sports competitions. Generally, these drugs are designed with therapeutic purposes, but they suppose a serious risk to athletes when used to enhance physical performance. Gene therapy is an experimental treatment that involves introducing genetic material into a person's cells to fight or prevent a disease. With the advances in gene therapy Gene Doping has become the biggest threat to sports.

As defined by the World Anti Doping Agency (WADA), Gene Doping is the "transfer of polymers of nucleic acids or nucleic acids analogues" and/or "the use of normal or genetically modified cells" with the potential to enhance sport performance.

Gene Doping has great potential because it can change gene expression drastically and permanently, and the doping substances are synthesized endogenously which makes its detection very difficult.

GENE DOPING DETECTION

The development of assays that are able to detect exogenous DNA in blood or urine is necessary. Gene Doping can cause health problems to athletes, in fact, gene therapy clinical trials have always had very controversial results and sometimes, side effects such as cancer or death have been reported.

There are two types of detection methods:

- Indirect detection methods: the human physiological response to gene transference or expression is measured. In these kinds of methods the immune response, the proteomic expression profile or RNA molecules are assessed.
- Direct detection methods: Exogenous DNA sequences via PCR are detected. For gene transfer to be successful, cells are commonly transfected with complementary DNA. Thus, non-human exon-exon junctions are used as targets. The amount of research groups studying transgene direct detection methods is bigger than those investigating the indirect ones, probably because they have more sensitivity and specificity.

However, according to WADA, currently there is no completely effective or reliable Gene Doping detection method.

Therefore, we propose a new qPCR-based direct detection method of the genes susceptible of being used in Gene Doping, for example *EPO*, *PPARD*, *HIF* or *GH*. In the same PCR reaction, sequences of genes associated to sports and some other neutral sequences of the human genome will be amplified. Then, the ratios of these two types of sequences during the career of the athletes will be compared. Any strong variation in the ratio would be suspicious of Gene Doping. The main advantage is that the method does not depend on targeting exon-exon junctions.

Methodologies like this are crucial to prevent the athletes from suffering health problems related to gene therapy side effects. Moreover, anti-doping policies help in restoring the confidence in sports.

An Online Interactive Tool to identify misconceptions in Genetics Education and promote a Conceptual Change

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KEY WORDS: Educational Innovation Project, misconceptions, interactive tool, Genetics Education, Didactic Material, Conceptual change

Genetics is a science in expansion whose applications are transmitted through the means of communications. It makes necessary a scientifically literate society able to 1) understand the fundamental concepts of this area, and 2) assess its ethical and sociological implications.

The study of Genetics is considered one of the most complicated didactic issues of Biology for Secondary School students and the general adult population. Publications of educational journals like *Life Science Education* have shown that misconceptions in Genetics have been detected through all the educational levels, even in university students and science teachers.

Last year, members of the Sport Genomics Research Group worked in the Master's thesis entitled *Identification and Analysis of misconceptions in Molecular Heritage in the Basque Country*. This project revealed that Secondary School students of our population have many bibliographically identified misconceptions in Genetics. Some of these alternative concepts persist in Bachelor. The results also showed a tendency to improve the assimilation of Genetics concepts when innovative teaching methodologies were used. In these methodologies 1) the student is the principal agent of the teaching-learning process, and 2) New Technologies and Communication Science tools are used in the development of teaching materials.

Following our previous research, we are carrying out an Educational Innovation Project (PIE) funded by the Educational Counseling Service of the University of the Basque Country UPV/EHU (SAE-HELAZ). Our aim is to develop and implement an online interactive tool to improve the active and independent learning process of Undergraduate students. To achieve this, the PIE has the following specific aims:

- To design and implement an accessible interactive tool to identify Misconceptions in basic Genetics of Undergraduate, Bachelor and Secondary school students of the Basque Country.
- To design specific educational didactic material to remove misconceptions in Genetics.

The work plan that we have designed for the implementation of this PIE between 2015 and 2017 includes these main features:

- Selection of Fundamental Genetics Contents based on the competences in the Basque curriculum of Secondary and Bachelor Students, and teaching guides of University Degrees with Genetic base. Likewise, those guidelines are contrasted with *Genetics Concept Inventories* and *Conceptual inventories Assessments in Genetics*.
- Identification of all existing conceptual errors in our population, using a literature review and open questionnaires with open questions. These preliminary results will be later used as item distractors in the final online evaluation tool.
- Development of an interactive, valid and reliable assessment tool following the guidelines set by Doval & Renom (2010) and the *Standards for Educational and Psychological Testing* (2014). Thus, the results will be assessed based on Bloom's Taxonomy.

Understanding disorders of the visual system and promoting repair and regeneration

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KEY WORDS: visual system, eye, repair, regeneration, GOBE.

The GOBE (Grupo de Oftalmo Biología Experimental) www-ehu.es/GOBE is a multidisciplinary research group interested in eye research. The group is integrated by ophthalmologists, biologists, physicists and veterinarians. Currently, GOBE have 10 members: 7 doctors and 3 PhD students.

The director of the group is Prof. Elena Vecino from the Faculty of Science and. The laboratory is placed in the Faculty of Medicine in the Dept. of Cell Biology and Histology. The group is a consolidated group that has been collaborating for more than 20 years in which has been formed Doctors Ophthalmologist that work in Hospitals such as Cruces, San Eloy, Donostia and Txagorritxu. The members of the group are also attached to Biocruces, Biodonosti and BioAraba. And collaborate with national and international groups in Universities of Munich, New York and Cambridge among others.

The methods and techniques that we use include animal models of glaucoma, primary cell culture, immunohistochemistry, proteomic, lipidomic, electron microscopy, use of biomaterials etc.

Our objective is to understand the cellular and molecular basis of a disease with the idea of future clinical applications.

The group have 4 principal lines of research:

1-Neuroprotection and Glaucoma (Prof. Elena Vecino). The retina is composed of groups of highly specialised cells that convert light energy into visual signals. Retinal ganglion cells (RGCs) collectively transmit visual information from the retina to several regions in the brain. Glaucoma is a neurodegenerative disease and cause leading of irreversible blindness that it is caused by the death of RGCs. Retinal glia cells are supportive cells and their relationship with ganglion cells is important for normal function, and by studying the molecular interactions between RGCs and glia, we hope to understand how we can prevent cell death.

2- Ocular Surface (Prof. Juan Durán and Dra. Arantxa Acera). The main objective is identifying biomarkers in tears, as a source of information for the ocular surface in different diseases with the idea to design artificial tears that could promote the repair of the injured ocular surface.

3- Analysis of aqueous humor in glaucoma (Prof. Haritz Urcola). Aqueous humour is a transparent, gelatinous fluid that is located in the space between the lens and the cornea. Lack of circulation of aqueous humour is one factor that increases intraocular pressure in glaucoma. We analyse the biophysical properties of aqueous humour in patients with glaucoma to detect changes compared with healthy eyes. Alterations in its composition may help us understand more about how glaucoma progresses

4- Uveitis (Dr. Alex Fonollosa) Uveitis is a term describing a group of inflammatory diseases that produces swelling and destroys eye tissues. This line studies cultured cells to test the possible action of somatostatin in the tight junctions formed in the retina-pigment epithelium with the aim of developing clinical applications. Moreover we are testing the effect of anti-inflammatory substances in different ocular tissues in vitro.

The role of the environment in the spread of antibiotic resistance genes

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KEY WORDS: metal pollution, organic amendments, phytoremediation, conjugative plasmids, antibiotic resistance.

Infections caused by multiple antibiotic resistant pathogenic bacteria have become one of the most important health problems. More than 70% of the bacteria causing nosocomial infections are resistant to multiple antibiotics, making treatment of such infections highly problematic. Therefore, there is an urgent need to develop new antimicrobial strategies to control infectious diseases.

The problem relays on the dissemination of the antibiotic resistant genes among bacteria by conjugative and/or mobilizable plasmids. Therefore, to find a solution it is necessary to understand the role of these genes and how they disseminate in clinical and nature environments. Since bacterial conjugation is the main mechanism responsible for the acquisition of antimicrobial resistance, our proposal aims at inhibiting the spread of antimicrobial resistance among pathogenic bacteria through inactivation of a key protein in the conjugative process. In this regard, our group is focused on the study the molecular mechanism of different proteins involved in bacterial conjugation as the first step to find a solution to the problem of antibiotic resistance spread.

Agricultural soil bacteria are subjected to high concentrations of antibiotic due to amendments with manure. This environmental pressure promotes the dissemination of antibiotic resistance genes among these bacteria. Analogously, since heavy metal resistance genes are also associated to conjugative plasmids, mine soil bacteria share conjugative plasmids among them. Therefore, both soils represent an ideal source to find conjugative plasmids to study different conjugative mechanisms. In this project we focused on the search of new conjugative plasmids from environmental unique soils in which both high concentrations of antibiotic and heavy metal are present.

Angelman Syndrome and Ubiquitination pathways

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KEY WORDS: neuronal disease, ubiquitin, biotin

Angelman Syndrome (AS) was first described in 1965, but its cause being a missing or mutated maternal contribution of the UBE3A gene, located on chromosome 15q, only discovered in 1997. The molecular basis for this pathology was however not any clearer after the discovery, since the product of the UBE3A gene is an ubiquitin E3 ligase responsible of the attachment of ubiquitin molecules onto its target proteins. E3 ligases can have multiple substrates, and therefore the manifestations of AS could be caused by the misregulation of any of the neuronal substrates of UBE3A. Despite its involvement in many physiological and disease-related processes, ubiquitination usually targets just a small fraction of any given protein, and it is still very challenging to identify this post-translational modification from human samples. The lack of a mammalian model system for both in vivo identification and validation of ubiquitination targets, has meant that several candidate UBE3A substrates reported during the last decade were only validated in vitro, with later in vivo studies contradicting the earlier conclusions. A review of the current state of the field will be presented, including advances by our lab.

FISIKA ETA INGENIERITZA ELEKTRONIKA

FÍSICA E INGENIERÍA ELECTRÓNICA



Early Universe Simulations

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KEY WORDS: Cosmic defects, cosmic microwave background, effective models, numerical simulations.

During the phase transitions that the Universe underwent, topological defects may have been created, typically giving rise to complicated defect networks. The understanding of the cosmological evolution and statistical properties of these networks are of utmost important in order to extract predictions from models of the physics of the Early Universe. Due to the high non-linearity of the behaviour of defects, it is essential to revert to numerical simulations. Thus, using numerical simulations, we can reproduce and describe the evolution on such exotic objects in the expanding universe.

In this talk we will firstly describe topological defects and their measurable effects, such as their imprints in the cosmic microwave background and the creation of gravitational waves. Then we will explain the numerical simulations we need perform to obtain that information. Finally, we will describe briefly the main aspects of the projects that we are working on at the moment:

- Analysis of the properties of Abelian Higgs cosmic strings networks and the characterisation of their possible cosmological signals (CMB anisotropies) using the biggest simulations ever performed in this area.
- Calibration of effective models using field theory simulations made in supercomputers.

Large Scale Structure of the Universe and Bose-Einstein Condensate Dark Matter

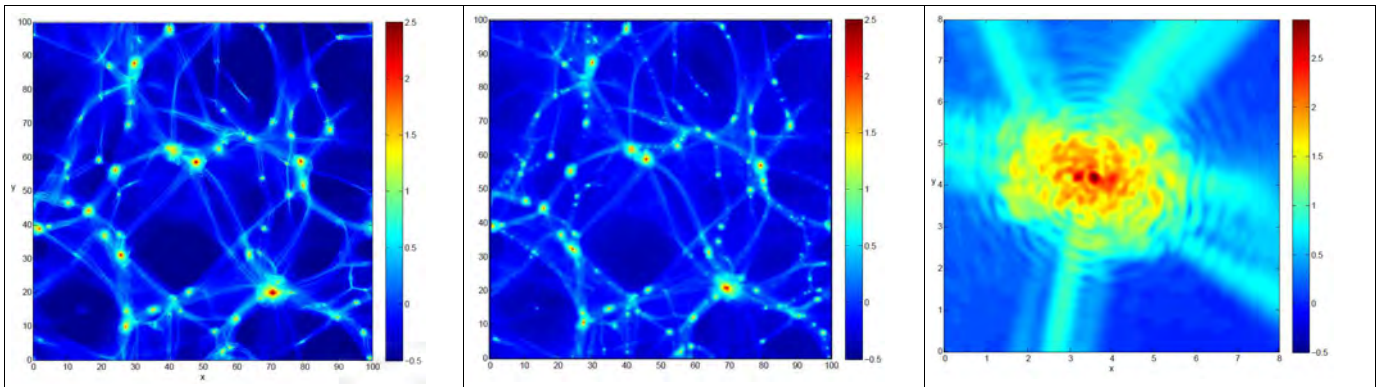
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KEY WORDS: cosmology, astrophysics, dark matter

Over the past decade increasingly reliable predictions of standard particle-CDM have been established by many independent groups with impressive N-body simulations which agree well with the large scale distribution of galaxies in the local Universe. After the inclusion of a cosmological constant, Λ , the standard Λ CDM cosmological model has no serious contender at present. Despite this success, there is of course deep concern that no dark-matter particle has actually been discovered, and with doubts now emerging from laboratory searches regarding the favoured candidates from super-symmetry theory. On astronomical scales, there is also tension on several fronts, including the smooth central densities of dark matter inferred from the slowly rising radial rotation curves of dwarf galaxies, whereas a central density cusp is predicted for standard particle-CDM. Furthermore, the observed numbers of dwarf satellite galaxies falls well short of the prediction of the Λ CDM cosmology. Arguably, Λ CDM is also in difficulty accounting for the surprisingly high speed collisions observed between pairs of galaxy clusters, including the Bullet-cluster and other subsequently discovered cases, where high relative velocities of 2000-3000 km/s are inferred for the colliding dark matter.

It may be reasonably argued that dark matter, such as axions or other lower mass scalar field particles, are perhaps even better motivated than the favoured dark-matter candidates from super-symmetric theories that remain undiscovered at the highest energies reached to date. Recent advances in string theory have opened up the possibility of an “axiverse”, with many light weight axions inhabiting the “dark sector” with a wide spectrum of masses. A characteristic feature of light scalar fields is that the associated bosons can form a coherent Bose-Einstein condensate under suitable conditions of temperature and density, and which can be met in the cosmological context. This fascinating state of matter, predicted by Einstein in 1925, has been observed for the first time in 1995 in experiments with ultracold trapped gases and is the subject of intense investigation.



Caption. Here on the left is shown the first simulation of large scale distribution of structures calculated for the case where CDM is in Bose-Einstein form (for a 100Mpc^3 box). Comparison with regular particle-CDM is shown in the center, demonstrating that the large-scale pattern of filaments and clusters is very similar. This is desirable as we know that the large scale distribution of matter is in very good agreement with standard CDM. Notice also the lack of small galaxy sized over-densities in the BEC simulation, compared to standard CDM, suppressed by the effective quantum pressure of the condensate, shown on the right.

Neutron stars in General Relativity

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KEY WORDS: stars: neutron, stars: rotation, methods: analytical.

A neutron star is a compact object that results from a supernova process of an original star that is, at least, 8 times more massive than the Sun. Neutron stars are known to be the most dense stars in the Universe: an average one contains 1.4 Solar masses packed in a sphere of radius 10 km. Their density is of the same order of magnitude of the density of an atomic nucleus! Another relevant magnitude is their angular momentum. Neutron stars rotate very rapidly: some of them with a period of tens of milliseconds (the period of the Sun is about 25 days). Due to the high density of neutron stars and their fast rotation, the Newtonian theory of gravity is no longer valid to describe their gravitational effects. In order to do that properly, we have to resort to General Relativity (GR).

The original relativistic treatment of rotating compact stars in equilibrium is due to Hartle, back in 1967. It constitutes the basis of most of the analytical approaches and is widely used to construct numerical schemes in axial symmetry. Hartle's scheme depicts the equilibrium (stationary) configurations of rotating isolated compact bodies in perturbation theory up to second order in GR. "Isolated and compact" means that the star finishes at a surface that separates its perfect fluid interior from a vacuum exterior, which is assumed to be asymptotically flat (the gravitational field decays to zero as one moves away). The perturbative scheme is based on a spherical (non-rotating) background configuration (a ball in vacuum), on top of which first and second order stationary and axisymmetric perturbations are computed. Hartle's model carries some explicit assumptions, which are expected to hold eventually in most cases. The perturbations are driven by a set of four functions that computed from the interior given an equation of state and conditions at the centre, are used to obtain the frame dragging effect, the deformation, and the total mass in terms of the central density and the rotation of the star. The model is constructed upon another implicit premise: the continuity across the surface of the star of those functions driving the perturbation, in terms of a particular coordinate system. However, in GR, this implicit assumption may subtract generality to the model. Worse, it could turn out to be a wrong choice, and lead to wrong outcomes.

In order to establish up to which extent the original "continuity" assumption had any consequence, or none at all, we have revisited Hartle's model within the general and consistent theory of perturbative matchings to second order by Marc Mars (USAL). We proved that the values of the functions driving the perturbations can be set to coincide on the surface, as assumed originally, except for one at second order. The discontinuity of this function contributes to the calculation of the total mass of the rotating configuration. The original expression of the mass, therefore, has to be amended: while the standard neutron star models are not affected by this correction, rotating star models (based on Hartle's scheme) with non vanishing energy density at the surface, such as homogeneous stars or strange quark stars, are affected and need a re-calculation of the curves representing the mass in terms of the central density. We have computed those curves for the homogeneous star model, completely described by Chandrasekhar & Miller in their classical paper, and we have found that the contribution of the amending term to the mass is far from negligible.

Finally, the perturbative matching is computed in our work on a purely geometric setting in a first step, without using any field equations. This can be used in more general situations, such as other theories of gravity for which Hartle's model has been generalised already in the literature, to find corresponding corrections to the mass.

Spin and relativistic effects in electron-phonon interaction and response functions of surfaces with strong spin-orbit coupling

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KEY WORDS: Computational Many-Body Physics, Spin-orbit coupling, Electron-Phonon coupling.

The main goal of theoretical condensed-matter physics is to understand and predict properties of materials, starting at the first-principles microscopic level: the quantum mechanics of electrons and atomic nuclei.

Treating many-body systems theoretically is a challenging task, requiring complex mathematical tools, as well as high performance computing. In our group we develop efficient methods, implementing novel theoretical techniques and numerical methods.

We are specially interested in surfaces composed of heavy atoms, in which inversion-symmetry breaking together with strong spin-orbit coupling (SOC) introduces new and interesting physics arising from the significant spin-splitting of the surface-state bands, as well as from the complex non-collinear spin textures.

Our main focus is on the response function and electron-phonon coupling (EPC) of such surfaces, seeking effects like charge and spin plasmons, and phenomena related to the theory of electronic transport and superconductivity.

Shortcuts to adiabaticity in the double well

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KEY WORDS: adiabaticity, double well, shortcuts.

The “adiabatic” concept may have two different meanings: the thermodynamical one and the quantum one. In thermodynamics, an adiabatic process is the one in which there is no heat transfer between system and environment. In quantum mechanics, as stated by Born and Fock (1928) in the adiabatic theorem: “a physical system remains in its instantaneous eigenstate when a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian’s spectrum”.

Here, we shall always understand “adiabatic” in the quantum-mechanical sense. Quantum adiabatic processes are in principle useful to drive or prepare states in a robust and controllable manner, and have also been proposed to solve complicated computational problems. However, they are prone to suffer noise and decoherence or loss problems due to the long times involved. This is often problematic because some applications require many repetitions or too long times.

Shortcuts to adiabaticity (STA) are alternative fast processes that reproduce the same final populations, or even the same final state, as the adiabatic process in a finite, shorter time.

Many of the existing approaches to design shortcuts, and even new ones have been used in the double well potential. These techniques have allowed us to obtain a great benefit in processes as varied as matter-wave splitting, multiplexing/ demultiplexing, beam splitters, cotunneling, population inversion, waveguide optimization, Tonks-Girardeau gas manipulation and bias inversion.

Theory of nanophotonics: Controlling light at the nanoscale with plasmonic nanoparticles

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KEY WORDS: plasmon, metal nanoparticle, nanoantenna, electromagnetic field, light

Thanks to the significant advances of fabrication techniques in the last decades, it is now possible to realize systems including nanosized components with a control of few tens of nanometers in size and geometry. This achievement has paved the way for the manipulation of light below the diffraction limits: indeed, metal nanoparticles are able to convert Visible-Near-Infrared light into collective excitations of conduction electrons at the nanoscale, called plasmons. At light wavelengths resonant with the plasmon, the metallic structures feature a remarkable absorption, despite their nanometric size, and an intense electromagnetic field enhancement and localization in proximity of their surface (accompanied by a notable temperature increase). For this reason metallic nanostructures are often referred to as nanoantennas.

Within this framework, we try to shed light on how to describe the phenomena taking place between nanoantennas separated by nanometric gaps. As a matter of fact, the plasmon-induced intense electromagnetic field is further enhanced in intermediate regions between antennas with nanometric separation, so called hot-spots. However, when the gaps are shrunk down to the nanometer, not only do other phenomena start to play a significant role (e.g., tunneling), but also the commonly used classical description does not hold any more and a quantum description is required [1].

The plasmon-excitation can also be exploited in combination with other optical effects. For instance, under the application of a static magnetic-field, magneto-optical (e.g., nickel) nanoantennas give rise to a component of the electric field in a direction orthogonal to the incident one. When the nanoantennas are placed in a periodic structure, the new component is not only enhanced due to the plasmon but also significantly modulated by the diffractive coupling introduced by the periodic arrangement [2].

Metal nanoantennas can also be effectively combined with phase-transition materials, such as materials whose optical properties change abruptly on a temperature basis (e.g., vanadium dioxide) [3]. Thanks to the plasmon-induced enhancement of the electromagnetic field it is possible to modulate down to the nanoscale the spatial temperature distribution in a phase-transition material, thus obtaining an all-optical active control of the material properties.

The theoretical study of this plasmonic light-matter interaction, spanning from the understanding of the key-mechanisms to the prediction of the induced phenomena, is of paramount importance for steering future efforts in the realization of effective electronic and optical nanodevices, such as molecular sensors, all-optical switches and thermal memristors.

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Magnetic and Structural Characterization of magnetic nanoparticles synthesized by *M. gryphiswaldense* bacteria

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KEY WORDS: Magnetic nanoparticles, magnetosomes, magnetotactic bacteria, magnetite.

Magnetic nanoparticles are subject of intensive research due to their interesting properties suitable for many innovative applications such as biomedical applications [1]. In this sense, magnetite nanoparticles are worthy mentioned due to their high magnetic susceptibility and biocompatibility. For that, last years have been witness to the development of numerous techniques focused on the synthesis of magnetite nanoparticles. However, one of the main challenges that chemical synthesis face is the control of the stoichiometry, the size or the shape of the magnetic nanoparticles. All these factors determine the final properties of our particles, and therefore, their possible applications.

A little explored synthesis methods are the synthesis of nanoparticles by biological routes. Magnetotactic bacteria synthesize magnetite nanoparticles with a high structural and chemical quality. The highly biologically control imposed in the synthesis determines the main properties of the particles like size, shape and magnetic properties. Depending on the magnetotactic bacteria specie we can find different sort of nanoparticles. Moreover, these magnetic nanoparticles, also called *magnetosomes*, are surrounded by a 2-3 nm lipid bilayer which make them more biocompatible and easier to be functionalized, which is ideal for biomedical applications[2].

The *Group of Magnetism and Magnetic Materials on the University of the Basque Country* works with the magnetotactic bacteria *Magnetospirillum gryphiswaldense* which synthesize cubo-octahedral magnetite nanoparticles of 45 nm nanometers with a narrow size distribution. By means of magnetic and structural characterization we are able to perfectly characterize these nanoparticles [3]. Microscopy techniques allow us to analyze the morphology and size distribution of nanoparticles. Moreover, thanks to the High Resolution *Transmission Electron Microscopy* (TEM) we are able to determine the crystalline structure of them, corresponding to the expected for magnetite. *X-ray absorption spectroscopy* (XAS) performed in synchrotron facilities (ALBA, ESRF...) gives us information about short range structure, probing again that our nanoparticles are clearly pure magnetite. Magnetic measurements such as hysteresis loops or *M(T)* complete the characterization of the nanoparticles.

Even though the enviable properties of magnetosomes make them really interesting for different applications, the lack of tunability of their properties could be a limitation. In order to extend the range of possibilities, last year we have been focus on the synthesis of doped magnetosomes by biological routes. In this sense, we have achieved to doping magnetosomes with Mn and Co just by adding these elements to the growth medium. The presence of the new elements has been checked with the already mentioned techniques.

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System-on-Chip (SoC) Applications: Intelligent Transportation Systems

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KEY WORDS: advanced driving assistance systems (ADAS), smart cars, embedded systems.

In the context of present challenges for society the aim of the Intelligent Transportation System (ITS) sector is mainly concerned with safety and wellness of drivers and passengers. The objective of this research line consists in extending “ambient-intelligence” concepts and technologies to “smart cars” using a driver-centred perspective where comfort, safety, and well-being are priority values. In particular, we focus on assisting the drivers with the aim of improving their awareness and driving performance in a non-intrusive way.

The availability of advanced driver assistance systems (ADAS), inspired in safety and well-being, is becoming increasingly important to avoid traffic accidents caused by fatigue, stress, distractions or chronic diseases, especially since the driving population is getting older. We investigate the suitability of driving behaviour signals, mainly CAN bus signals and pedal-sensor recordings (e.g. gas pedal pressure, brake pedal pressure, vehicle velocity, etc.), to develop models of the drivers’ behaviour in different environments (highways and roads), and performing different driving tasks, with the aim of identifying anomalous driving situations and warning the driver about it. These signals are obtained in a nonintrusive manner, without disturbing the driver -as opposed to speech-signal based methods; the group is using data obtained with the “Uyanik” instrumented car (University of Savanci, Istanbul).

DEVELOPMENT OF SoCs FOR DRIVING ASSISTANCE SYSTEM IMPLEMENTATION

An embedded system is a special-purpose computing platform designed to perform one or several dedicated functions. They are often designed for a particular kind of activity that is required to work under certain constraints, such as low power consumption, real-time operation, processing capacity, dependability or security. In addition, low cost, and small size/weight are also typical requirements for these computing platforms.

The automotive sector has taken advantage of field programmable gate arrays (FPGA), mainly due to the high computational demands of this sector where a huge amount of signals have to be processed in “real time” by means of very fast electronic systems. Currently FPGAs are used as embedded platforms (SoPC) or hardware coprocessors for algorithm acceleration, and as sensor interfaces (camera sensor interface, infrared or thermal camera interface, radar sensor interface, CAN bus interface, etc). The main objective of this research line is the development of embedded electronic systems, based on FPGAs, for in-vehicle deployment of ambient intelligence with the aim of improving driver performance and safety in an unobtrusive manner. This objective is an innovative and multidisciplinary approach for the development of ADAS which involves the following partial research objectives:

- To develop driver identification and driver status identification models based on behavioural signals obtained in a nonintrusive way and suitable for digital hardware implementation.
- To implement efficient real-time electronic systems for the above models using FPGA-based embedded systems for in-vehicle integration.
- To develop practical implementations of ADAS in order to verify and enhance the proposal, to determine their feasibility, and to propose alternative solutions.

GEOLOGIA

GEOLOGÍA



Human impact in Suances (Cantabria) estuary: geochemical and microfaunistic indicators in the current sediments

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KEY WORDS: sediments, estuaries, Anthropocene.

Metal and benthic foraminiferal contents from 22 surface sediments and 1 core (8 m) in the Suances estuary have been analyzed in order to characterize the geochemical and microfaunal responses to the recent environmental conditions in this coastal area.

High levels of Zn, Pb and Cd together with reduced numbers of foraminifera (dead and alive) present in this estuary suggest very negative and persistent environmental conditions through time as a consequence of mining, industrial and urban effluents disposal in this ecosystem during the last 160 years.

Multiproxy geological analysis represents a powerful tool for the historical monitoring of both the past and future environmental transformation processes.

Multi-isotopic studies used to reconstruct residential mobility and diet of North Spain Medieval populations

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KEY WORDS: stable isotopes, radiogenic isotopes, palaeomobility, dietary patterns, Medieval populations, North Spain, teeth, bones.

Stable isotopes ($\delta^{13}\text{C}$, $\delta^{15}\text{N}$, $\delta^{18}\text{O}$) and radiogenic isotope ($^{87}\text{Sr}/^{86}\text{Sr}$) are used to characterize migration events and diet patterns of past populations. These studies are increasingly important in archaeological, cultural, social and forensic applications. Carbon and nitrogen isotopes composition in bone collagen constitutes an important approach to palaeodietary reconstruction. They provide information about the protein consumption averaged over at least the last 10 years prior to death and also about the protein food sources. On the other hand, strontium and oxygen isotopes are used to identify migrant individuals and to reconstruct the mobility of past populations. These isotopes correspond to two independent isotopic systems, where strontium reflects the geological region while oxygen reflects geographical area of provenance of individuals. The combination of these two isotopes provides information about birth area of individuals and migration patterns.

Identifying non-local individuals within the population of a community allows to study migration events, population mixture and population dynamics in the past. $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ studies reveal significant knowledge on food distribution within populations and the differences in diet based on sex, social status and age.

These isotopic studies are conducted based on several Medieval Age archaeological sites of North Iberian Peninsula between VI-XII centuries. Particularly three sites are considered, a Muslim archaeological site located in Zaragoza, a Christian archaeological site from El Condado de Trevino (Burgos), and a last archaeological site from Bizkaia consisting of Christians and Pagans individuals. Results show differences in diet according to age and sex of individuals, marking a social structure in the population regardless of religious beliefs. Dietary difference lies on the proportion of animal protein consumption, mainly adult male consumed more protein than female and young male. Regarding to individuals mobility during the Middle Ages, migrant individuals were usually female and young male.

Future studies will be focused on comparing these results with other medieval communities from the nearest geographical area as well as with more distant populations both from inside and outside of the Iberian Peninsula.

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Development of SOFC components

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KEY WORDS: combustion synthesis, SOFC components, SOFC commercialization.

ABSTRACT

Solid oxide fuel cells (SOFCs) have the potential to be one of the cleanest and most efficient energy technologies for direct conversion of chemical fuels to electricity. Economically competitive SOFC systems appear poised for commercialization, but widespread market penetration will require continuous innovation of materials and fabrication processes to enhance system lifetime and reduce cost. Additional requirements arise for the technologies for synthesis of SOFC materials. These requirements originate from the demands for large scale SOFC industrial production. In this sense, solution combustion synthesis (SCS) is a simple and reproducible method used to obtain several types of ceramic oxides for a variety of applications. A typical SCS procedure utilizes a self-sustained exothermic reaction among well-mixed reactants to achieve the rapid and economical synthesis of particulate products. Up to 2008, SCS method has been adopted to fabricate more than 1000 kinds of oxide powders over more than 65 countries [1]. The properties of the resulting powders (crystalline structure, amorphous structure, crystallite size, purity, specific surface area and particle agglomeration) depend heavily on the adopted processing parameters [2,3].

For these reason, we have synthesized different parts of a fuel cell, on a large scale, by the glycine-nitrate combustion method. It have been synthesized interconnector protective coatings ($\text{MnCo}_{1.9}\text{Fe}_{0.1}\text{O}_4$), contact layers ($\text{LaNi}_{0.6}\text{Fe}_{0.4}\text{O}_3$), cathodes ($\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_3$), interlayers ($\text{Sm}_{0.2}\text{Ce}_{0.8}\text{O}_{1.9}$), electrolytes ($\text{ZrO}_2)_{0.92}(\text{Y}_2\text{O}_3)_{0.08}$ and anode ($\text{Ni}_{0.3}\text{O}-(\text{ZrO}_2)_{0.92}(\text{Y}_2\text{O}_3)_{0.08}$) materials, obtaining reproducible pure samples and amounts up to 12 g for each batch, being able to increase easily this amount to lots of hundred of grams. The obtained materials have been characterized compositionally by inductively coupled plasma atomic emission spectroscopy (ICP-AES) and X-ray fluorescence (XRF), structurally by X-ray diffraction (XRD), microstructurally by scanning electron microscopy (SEM) and by conductivity measurements.

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Reversible structural transformation of a Cu^{II}-based solid coordination framework with 2'5-pyridinedicarboxylate and di-2-pyridyl ketone: Synchrotron radiation analysis

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KEY WORDS: MOFs, Synchrotron, Crystallization, DFT, SCFs.

ABSTRACT

Phase transformations in solid coordination frameworks (SCFs) are of interest for several applications, and this work reports on a crystal-to-crystal transformation found for a hydrogen bonded Cu^{II}-based solid coordination frameworks (SCF) [1,2]. Thus, combination of PDC and (py)₂C(OH)₂ ligands, where PDC is pyridine-2,5-dicarboxylate and (py)₂C(OH)₂ is the derivative gem-diol of di-2-pyridyl ketone ((py)₂CO), produces [Cu(PDC)((py)₂C(OH)₂)(H₂O)] (**1**). Compound **1** transforms into [Cu(PDC)((py)₂C(OH)₂)] (**2**) by thermally-induced dehydration. Characterization of both compounds has been carried out by means of IR spectroscopy, single crystal and powdered sample X-ray diffraction (XRD) through conventional and synchrotron radiation, thermogravimetry (TG), X-ray thermodiffractometry (TDX), and scanning electron microscopy (SEM). Since the molecules of water in **1** are coordinated to the metal ions, their removal provokes local distortions on the coordination sphere (square pyramidal for **1** and square planar for **2**), which extend through the whole framework affecting the hydrogen bond system and the packing. In fact, the wavy nature of the planes in **1** becomes sharper in **2**, producing an oscillation of the framework: i.e., from open (**1**) to close (**2**) waves. The crystal-to-crystal transformation is reversible (**1**⇌**2**) and hysteresis has been observed associated to it. Quantum-mechanical calculations based on the density functional theory (DFT) show that the **1**⇌**2** structural rearrangement involves a high amount of energy, meaning that the role of the coordinated molecule of water exceeds the mere formation of hydrogen bonds [3].

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MATEMATIKA

MATEMÁTICAS



Comparison of beta-binomial regression model approaches to analyze health-related quality of life data

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KEY WORDS: Beta-binomial regression, HRQoL.

Health related quality of life (HRQoL) survey data is usually presented in an ordinal form and, therefore, it is assumed to be distributed as a binomial random variable. Theoretical assumptions of the selected model and interpretation of the results are issues to take into account when selecting an appropriate statistical model to analyze HRQoL data. A quite general approach is to account for the over-dispersion of the data by means of the beta-binomial distribution.

Previous work showed that interpretation of the results based on a beta-binomial regression model was very convenient (Arostegui et al., 2007). Based on the literature, theoretical inference in a beta-binomial regression model could be approached in two different ways: i) response variable with a beta-binomial distribution and a logistic link function (Forcina and Franconi, 1988); ii) hierarchical likelihood approach (H-Likelihood) (Lee and Nelder, 1996). Comparison of both approaches has not been addressed from a practical point of view. Indeed, the logistic regression with over-dispersion is probably one of the most frequently used approaches when analyzing HRQoL data as response variable.

This work was motivated by the analysis of real data application of HRQoL outcome in patients with stable Chronic Obstructive Pulmonary Disease (COPD), where response variable was the Short Form - 36 (SF-36) Health Survey, which is one of the most widely used HRQoL instruments in clinical research. Patients' socio demographical and clinical conditions were used as independent variables in the modeling process. The use of both approaches yields to contradictory results in the estimation and interpretation of the covariate effects. A simulation study was performed to check the difference in results provided by both approaches under controlled conditions based on the shape of the random effects. Three different scenarios were considered, random effects that were bell-shaped, U-shaped and flat. We provide an explanation of the results in both methodologies and address the need to apply the proper approach in the analysis of HRQoL survey data for practitioners, providing an R package.

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Presentation of the Mathematical Technology Transfer research group of the UPV/EHU

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KEY WORDS: mathematical technology, statistical techniques, optimization.

The Mathematical Technology Transfer research group of the University of the Basque Country (UPV/EHU) is devoted to the mathematical modelling of some industrial processes as well as the development of some mathematical techniques that give rise to the solution of demands from Public Institutions. Mathematical formulation is used in order to obtain a better knowledge of the problem. Subsequently, data processing, statistical techniques and optimization algorithms are applied for characterizing the behavior of the variables and for optimizing the results.

SUBTITLE

Here we present three examples of mathematical models applied to practical problems coming from an industrial company, an Internet service company and a public health service.

The first example proposed consists on the search of the widest rectangular surface of usable wood on an irregular piece of lumber. This is a typical problem that appears in a sawmill. The coordinates of the lumber have to be measured by electronic devices and parametrized by geometrical variables. A formal solution of the optimization problem can be found by mathematical programming but the requirements imposed in order to have a low computational cost lead to an efficient heuristic algorithm.

The second example address the problem of finding an optimal itinerary. Given a map with a set of points, each one punctuated by a particular numerical prize, the aim is to pass through the most convenient points maximizing the accumulated scoring. It is imposed a restriction about the maximum length permitted on the itinerary. In this case genetic type algorithms are the most efficient to tackle the problem.

The last example deal with the management of the production and distribution blood platelet concentrate units on a blood transfusion center. Here the problem of inventory management is not trivial because this type of product is perishable and the production capability and the demand depends on the day of the week. Also seasonality effects add difficulties to the mathematical model. A statistical analysis of the demand helps definitively in the design of a strategy that optimizes the quantity of items to be produced each day giving rise to a considerable reduction of the out-dated items and the age of the transfused items.

Stochastic Optimization, Risk Management and High Performance Computing

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KEY WORDS: stochastic optimization, risk management, high performance computing, CPLEX, COIN-OR.

Stochastic Optimization is a field of Operations Research that appeared as a response to the need of including uncertainty in optimization models and it is broadly studied and applied in today's real-world applications. Uncertainty is the key ingredient in many decision problems. Basically, it deals with situations in which some parameters are random variables (i.e., coefficients in the objective function, the right hand side vector and the constraint matrix). It allows the risk inherent into the random variables of the problem to be managed, or at least partially managed.

In the general formulation of a multistage stochastic integer optimization problem, decisions on each stage have to be made stage-wise. Moreover, there have been few attempts to solve large sized multistage stochastic mixed 0-1 models up to optimality due to their complexity. When the main aim is the efficiency of the approaches, we can consider metaheuristic algorithms, such as Cluster Lagrangean Decomposition or Fix-and-Relax Coordination. When optimality is an imperative, Cluster Benders Decomposition or Multistage scenario cluster primal methodology can be considered. In any case, this type of problems require an intensive computing effort, even using decomposition algorithms for problem solving. Parallel Computing offers an alternative by parallelizing the solution of mixed integer submodels that appear in the decomposition algorithms and parallelizing the execution of some steps of the algorithms. We have implemented some algorithms for solving large sized multistage stochastic problems, as the parallel version of the Multistage Branch and Fix Coordination algorithm (P-BFC) and the Multistage Stochastic Dynamic Programming (P-SDP). The parallelization is performed at two levels, so-called inner and outer. The speed-up and the solution values improvement in the tested instances are remarkable.

The stochastic optimization models consider, in general, the optimization of the objective function expected value alone, so, the risk neutral (RN) environment is assumed. However, the optimization of the RN objective function has the inconvenience of providing a solution that ignores the variability of the objective function value over the scenarios. There are some approaches that additionally deal with risk measures in the more realistic risk aversion environment. Recently, new risk averse measures for two-stage stochastic mixed 0-1 problems have appeared in the literature, in particular, the so named first- and second-order Stochastic Dominance Constraint (SDC) recourse-integer strategies for a set of profiles included by pairs of thresholds on given function values and some types of shortfall related bounds on reaching them. We are studying the multistage time inconsistent mixture of those two SDC measures. Those approaches are more amenable than the classical mean-variance schemes. We study the risk aversion strategies in the applications using the decomposition algorithms so-named BFC-SDC and CLD-TSD.

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KIMIKA

QUÍMICA



Quantum Simulations with Trapped Ions

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KEY WORDS: quantum simulation, trapped ions.

Feynman conjectured that quantum computers might be able to simulate quantum systems in a more efficient way than classical computers. Even though universal quantum computers are not feasible with current technology, quantum simulators can be used for this purpose. A quantum simulator is a controllable quantum system that mimics the dynamics or static properties of a quantum model. There are two main types of quantum simulations: analog, when the quantum simulator dynamics is governed by a similar Hamiltonian of the simulated model, and digital, when the evolution of this simulated model is implemented by a quantum algorithm constructed by sequential unitary gates. Ion-trap quantum technology consists in the control and manipulation of single or multiple cold atomic ions that are trapped by means of electromagnetic fields. Lasers or microwave fields can be used to control two electronic levels of the ion that serve as a qubit. The motion of the ion is cooled down until it reaches the quantum regime. Currently, trapped-ion technology offers one of the highest degrees of controllability among quantum technologies, making it a good candidate for quantum simulation and quantum computation protocols. This quantum platform seems suitable for implementing digital-analog quantum simulations, a new approach developed in QUTIS, that employs digital techniques with analog interactions, which allows us to exploit the complexity of the simulating quantum systems.

Fluorescent hybrid materials for optical applications

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KEY WORDS: 1D-Aluminophosphate, dyes, Non-Linear Optics, color switching, white light.

Different dyes have been encapsulated into the inorganic host MgAPO-11 in order to obtain appropriate hybrid materials for optical applications. This zeolitic host with AEL structure-type has narrow one-dimensional elliptical nanochannels (with a diameter of $6.5 \times 4 \text{ \AA}^2$) which fit very tightly to the molecular dimensions of many organic dyes. The tight fitting prevents the molecular aggregation of the dyes and induce a preferential orientation along the nanochannels. However, due to the tight fit between the molecular and channel dimensions, the dye cannot be incorporated into the structure via post-synthetic methods; the dyes are encapsulated by crystallization inclusion method, or one-pot synthesis approach. In this method, dyes are added to the synthesis gel and get occluded while the inorganic framework crystallizes.

Thereby, occluding a dye with intrinsic Non-Linear Optical properties, the hemicyanine LDS 722, we obtained a very fluorescent hybrid material emitting in the red edge of the electromagnetic spectrum, reaching a fluorescence quantum yield fifty times higher than that for the dye in aqueous solution, owing to the rigidity imposed by the host matrix ($\phi_{\text{fl material}}$: 0.51 vs $\phi_{\text{fl aq.}}$: 0.001). Moreover, due to the high degree of ordering of the dye molecules along the c-axis of the nanochannels of the aluminophosphate, the material shows interesting second-order non-linear properties, such as second harmonic generation.

On a second step, two dyes were occluded in order to find a hybrid material interesting for dichroic applications. Acridine (AC) and pyronin Y (PY) were chosen as they have similar molecular structure, but with perpendicular transition dipole vectors, so that a complementary response to the linearly polarized light is expected. As a result, a fluorescent hybrid material with emission color switching was obtained with the polarization of the light, in which an efficient Fösters Resonance Energy Transfer (FRET) takes place from AC to PY. This energy transfer process is possible mainly due to the fluorescent properties of the donor, the spectral overlap between dyes and the high probability of energy transfer between neighbouring channels.

Finally, the relative proportion of the three dyes mentioned in the synthesis gel was optimized in an attempt towards the obtainment of White Light and for to improve the light harvesting capacity of the system. The resulting hybrid material from the optimized gel shows an emission that covers the whole visible spectrum, giving white fluorescent light, with CIE chromaticity coordinates close to ideal coordinates for white color.

MALDI IMS: Mapping Metabolites

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KEY WORDS: MALDI, Imaging Mass Spectrometry, Lipids, Lipidomics, Orbitrap, MS.

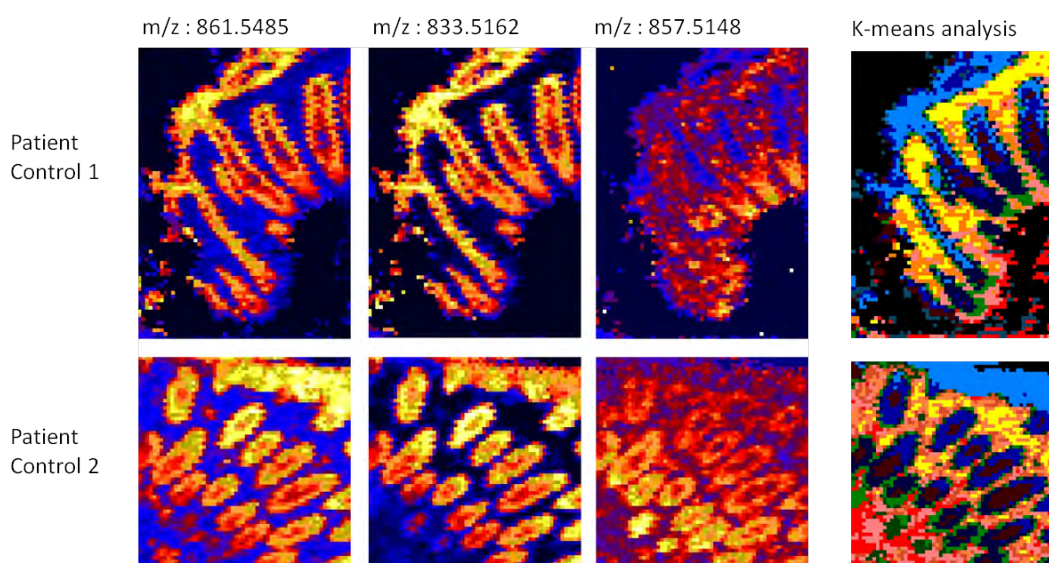
The “omic” studies involve large number of non targeted measurements (genes, proteins, lipids), which are chemical markers indicative of biological events (High-dimensional Biology). The main goal is to acquire comprehensive knowledge of biological processes not only in normal physiological state but also in different pathologies. One of the research lines in our group is the use of mass spectrometry in lipidomics to understand complex biological problems

Lipids play an important role at cellular and whole organism level and therefore there might be some alteration in different aspect of lipid metabolism that can affect numerous cellular processes causing diseases such as cancer.

Mass spectrometry has gained considerable relevance on lipidomics with Imaging Mass Spectrometry due to its ability to obtain the spatial distribution of lipids in tissue sections.

Advantages of this analytical technique are high sensitivity, robustness, high-throughput capacity and applicability to a wide range of molecules without damaging the tissue. Moreover, this method is label-free, so there is no need of any kind of chemical marker that could alter the lipidome of the tissue. But there are still a number of factors limiting its use. Challenges remain in the areas of higher spatial resolution, normalization, ionization method and quantification.

Here we present, as an example, lipid distribution of a human colon biopsies at cellular level (10-5 μm) using the oversampling technique on a commercial MALDI-LTQ-Orbitrap (Thermo) with an originally elliptical laser beam of 168x37 μm without losing signal intensity.



Microwave Spectroscopy: From essential sugars to Stars

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KEY WORDS: microwave spectroscopy, rotational spectra, sugars, astrophysical molecules.

Microwave spectroscopy is the most accurate technique to determine the structure of molecules of different nature in the gas phase. Its extremely high resolution (sub-Doppler) allows discrimination between the different species in the jet, whether tautomers, conformers, isotopomers and enantiomers.

Recently, our group has designed and built two different microwave spectrometers (non-commercial equipment): Molecular Beam Fourier transform microwave spectrometer (MB-FTMW) coupled with an ultrafast laser vaporization system (figure 1a) and a Chirped Pulse Fourier Transform spectrometer (CP-FTMW, figure 1b).

Our goals have been biomolecules (sugars, peptides, drugs...) and molecules of astrophysical interest. Here, we showed some studies on monosaccharides including ribose, fructose or 2-Deoxy-D-ribose have revealed that the most stable structure adopt for them in gas phase is the pyranose form while in the biological medium (RNA or DNA) that sugars are found in their five members ring structure. The experimental work was supported by theoretical calculations.



Figure: 1a. Set up of the LA-MB-FTMW.

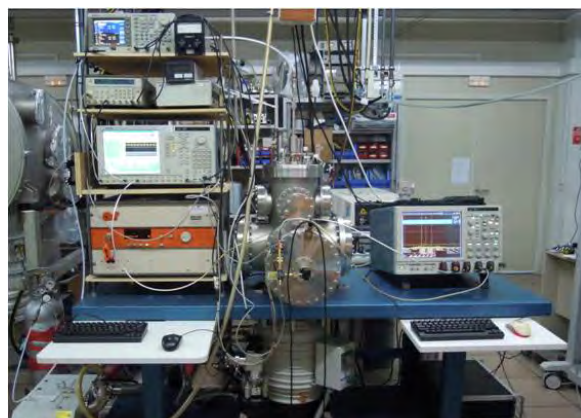


Figure: 1b. Set up of the CP-FTMW.

Laser Spectroscopy in Molecular Beams: a powerful tool to study biological systems

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KEY WORDS: Double resonance spectroscopy, Laser Spectroscopy, Molecular beams, Biological systems

Mass-resolved laser spectroscopy is a powerful tool in which classical spectroscopic techniques are combined with the advantages of laser radiation in order to obtain higher resolution than with conventional spectroscopic techniques. Furthermore, the use of mass-selective detection allows us to study complex mixtures and molecular aggregates. Combination of such techniques with molecular beams permits to deal with isolated molecules, removing the solvent effects, and to form molecular clusters, providing a good insight on the non-covalent interactions behind the formation of the aggregates. These non covalent interactions are essential in the stabilization of different biological system.

Our group has developed a sophisticated methodology to fully characterize molecular aggregates of biological relevance. This methodology includes a number of spectroscopic techniques: REMPI, 2-color REMPI, double resonance techniques, such as UV/UV hole burning, IR/UV, IR/IR/UV/UV and IR3, which allows us to tackle the mass-resolved IR spectroscopy of systems without a chromophore. Interpretation of the experimental information obtained using such techniques is not straightforward and requires of theoretical predictions to understand the conformational preferences of biological aggregates. The systems studied using this methodology include aggregates of DNA bases, xanthynes, sugars, drugs and their cross-aggregates. Some of the questions behind such studies include what are the real aggregational preferences of DNA bases in absence of any external perturbation. May be nature chose CGAT as the alphabeth of life because their unique combination of hydrogen bond and stacking interactions. Also we try to unravel how sugar units interact, to shed light on the mechanisms of molecular recognition involved in the function of the immune system.

Polymers: answers for XXI. Active surfaces

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KEY WORDS: Polymers, Advanced manufacturing, 3D-printing, shape memory, nanoparticles, ground remediation.

While the bulk properties of a material determine its mechanical performance, the interactions between the material and environment are governed by its surface properties. Consequently, the manipulation and control over the surface properties of a material, without altering its bulk properties, is crucial for producing materials of high added value. The European manufacturing enterprises and the European Union have determined the advanced manufacturing as one of the basic pillars of the European research for Horizon 2020 program. So, the fabrication of active polymeric surfaces could be considered as a key factor to obtain high-tech materials required for advanced fabrication.

Between the research lines of Macromolecular Chemistry Group of the department of Physical Chemistry of the Faculty of Science and Technology (UPV/EHU), one of them is focus in the development of Active surfaces.

BIOMIMETIC SURFACES

Nature has been using nanotechnology since the beginning of time to prevent infections, repel water or create colors. So, one of the actual scientific challenge is to generate nanometric structures inspired by nature. The nanoscale patterns on the shark's skins are good example of nature's structures; these nanostructures avoid the accumulation of barnacles, algae, and bacteria. A synthetic surface with this kind of arrays could provide the materials with a highly interesting antibiofouling properties.

BIOACTIVE SURFACES

Bioactive surfaces are surfaces with immobilized bioactive molecules capable to promoting or supporting particular interactions with biological compounds. This kind of surfaces has crucial importance in biomedical and biomaterials applications. A remarkable effort has been made to create bioactive surfaces by forming specific biomolecule-modified surfaces with antibiofouling properties

BIOSENSORS

Biosensors are electrical, optical, chemical, or mechanical devices capable to detect selectively biological species. An ideal biosensor is one that not only has the capability to respond to low concentrations of analytes, but also should have the ability to discriminate other species. The recognition of the specific analytes take place by their immobilization on biosensor's surface. Biosensors have wide applications such as medical diagnostics or pathogen and toxin detection in food and water.

Dried Blood Spot: The future of blood sampling?

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KEY WORDS: DBS; UHPLC-PDA-FLR; MALDI-LTQ-Orbitrap.

In this work, the reliability of Dried Blood Spot (DBS) as a sampling technique for drug analysis has been studied using Ultra High Performance Liquid Chromatography coupled to Photodiode-Array and Fluorescence Detection (UHPLC-PDA-FLR), and Matrix Assisted Laser Desorption source coupled to a tandem mass spectrometer ion trap /Orbitrap (MALDI-LTQ-Orbitrap).

DBS microsampling is a technique based on placing a drop of blood in a cotton support that is left to air dry. This sampling technique, used for the first time with human blood in 1963, has lately noticed an increase in use in bioanalysis thanks to the sensitivity improvement of the analytical methods.

DBS sample treatment is straightforward: firstly, blood is collected by a finger, heel or ear prick and spotted in the DBS commercial cards. Secondly, after drying (from 3 to 8 hours at room temperature) the spots are punched out and extracted by a solid-liquid extraction. In this work we used as extraction solvent methanol: pH 2 phosphate buffer (75:25) solution assisted by sonication and centrifugation. Finally, the extracted compounds were analyzed.

DBS technique offers several advantages compared to common blood sampling methods: a higher stability of the analytes in the support, a smaller sample volume, an easier and cheaper sample storage and transportation, and a lower biohazard risk. However, it also shows some limitations for quantitative analysis due to the dependence on different factors. The influence of the most significant variables as hematocrit, blood volume and sampling position on the quantitative response was investigated using amiloride, propranolol and valsartan drugs as model compounds. These drugs were analyzed by UHPLC-PDA-FLR.

It was observed that this sampling technique allows a simple and fast analysis of different drugs simultaneously. According to the results, it was concluded that the sampling position and the hematocrit have influence in the accuracy and precision of the quantitative results, therefore limiting the use of this technique. On the other hand, the analysis of the analytes dispersion was studied by UHPLC-PDA-FLR and MALDI-LTQ-Orbitrap. Based on the results obtained, it was proved that the dispersion of the analytes depends on their physicochemical properties. In this way, the distribution of each analyte must be carefully studied during the method development for a more reliable quantification.

Contributions of microencapsulation in environmental health

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KEY WORDS: microencapsulation, volatile bioattractants, environmental health

The search of alternative methods associated with the problems of environmental health is one of the great challenges of this century. The advantages of the pesticides microencapsulation process as decrease of toxicity, increase of handling security and increase of solubility in water, represent a good option to face the environmental health problems. Microencapsulation consists of an active compound is surrounded with a wall avoiding the direct contact with outside. In order to optimize a microencapsulation process, the application of final product should be defined, the release of the active compounds, the different kind of chemical encapsulating agents used, physical and chemical properties of the guest, size of particle required and the cost of the process should be considered.

A bait for insects used in indoor places, such as schools, companies or hospitals was developed. The encapsulating agents tested were cyclodextrins utilizing a fast procedure of microencapsulation with a high efficiency. The size of particles must be the smallest to minimize detection of the insects and to treat a larger surface area. The particles have to be smaller than 100 μm , but in the same way it has to be bigger than 20 μm to decrease the toxicity for breathing and to avoid the loss for evaporation. In this study, the size of particles was 50 μm . Finally, the cost of the procedure will be low because the work time is short and only it is employed water, which makes the process environmental friendly.

The research group previously has studied and analysed qualitatively and quantitatively some volatile compounds from a variety of fungi and these are attractant of some species of insects. In this work volatile bioattractants and pesticides have been microencapsulated to give rise to a bait, getting a more specific and selective product which only affects to a specific species of insects and does not change the natural life of the animals.

To monitorise the release of bioattractants from the encapsulated product at room temperature, a static headspace analysis by gas chromatography-mass spectrometry (HS-GC/MS) method was well optimized and validated with good results in selectivity, linearity, accuracy and precision.

Schizophrenia: A challenge for Metabolomics

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KEY WORDS: Schizophrenia, Metabolomics, Features.

Schizophrenia is a multifactorial neuropsychiatric disease that affects about 1% of the general world population and generally appears in early adulthood. This psychiatric disorder is influenced by both, genetic and environmental factors. It is a socially known illness, but its metabolic pathways or involved molecules are still unidentified. This fact causes the absence of objective tools to diagnose, and therefore, it must be done by a clinical specialist based on psychiatric manuals that makes the diagnosis less subjective. However, even with these manuals, the number of errors in the diagnosis is very high, confounding it with other psychiatric diseases as bipolar disorder or lazy personality of a healthy person. Another problem linked to the lack of knowledge of the biological routes implicated in schizophrenia is the treatment provided to the patients, which is normally non-specific because the selection of the appropriate antipsychotic drug is done taking into account the effects caused.

The omic science Metabolomics can be defined as that which studies the metabolome, this is, the group of all metabolites or small molecules (<1200 Da) in a certain organism. The metabolites are compounds with different physicochemical properties such as carbohydrates, amino acids, vitamins, lipids, steroids, etc. Metabolomics has the advantage with regard to the rest of omics (genomics, transcriptomics and proteomics), of being the nearest to the individual phenotype.

The aim of this work is the application of Metabolomics as a helpful tool to obtain useful information on the schizophrenia disease. Metabolomic profiles can help to find putative biomarkers of this disease which can be used for an early diagnosis. To carry out this objective blood samples were collected from 56 healthy controls and 56 schizophrenic patients and stored at -80°C until analysis. Protein precipitation with cold acetonitrile was chosen as optimum sample treatment and liquid chromatography-mass spectrometry was used for getting the metabolomic profiles of plasma extracts. In this study, UHPLC-Q-TOF equipment was used with a C18 column and operated in positive electrospray (ESI+) ionisation mode. Pre-processing of data obtained was carried out using XCMS software that gives a data matrix with different matched features (pairs mass-to-charge ratio (m/z)-retention time (RT)). Then, the matrix was introduced in SIMCA software to do a multivariate statistical analysis and to detect discriminant features between groups. Finally, features identification was done based on the comparison of spectrometric signals with databases, as METLIN or HMDB, to allocate each feature with a certain metabolite. The results obtained in this study, doing an unsupervised analysis using principal component analysis (PCA), indicate a separation tendency between the two groups studied: schizophrenia patients and healthy controls, which is clearly corroborated by supervised analysis. From the OPLS-DA model, it can be found some features that discriminate both groups, with a total of 3 up regulated features in healthy controls and 10 in schizophrenia patients. The future research will consist of identifying the features that differentiate the groups studied and to find the biological pathway where metabolites are involved.

Short term stability of the extracts of 22 emerging contaminants in different supporting media

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KEY WORDS: Stability; emerging and priority pollutants; aqueous samples; polymeric materials; polymer characterization

Many synthetic organic chemicals are produced and used in large quantities worldwide for different purposes and, consequently, they are continuously released into the environment. Persistent organic pollutants (POPs) or priority compounds are today less relevant for the industrialized countries since a drastic reduction of emission rates has been achieved due to the implementation of appropriate policies and regulations and the gradual elimination of the main sources. However, a growing concern is observed when the “emerging” or certain unregulated contaminants are considered as a consequence of the uncertainties about their effects and risks for the environment and human health.

Water sample analysis usually requires short term storage to manage the processing of a large number of samples. Consequently, it is important how to assure the integrity and stability of these samples before being processed. Labile analytes such as pharmaceuticals and pesticides are bioactive and hence may undergo different chemical, physical and biological processes between sampling and analysis. Thus, depending on stability, quantifying a compound that has been excreted several hours previously may, in fact, lead to a significant over or under estimation of the actual amount of residue originally present. Currently, since no uniform way of sample collection and handling different approaches have been reported in the literature

This work describes a stability study performed in seawater spiked with 23 emerging and priority compounds belonging to 9 different groups: herbicides, hormones, stimulants, artificial sweeteners, personal care products, phytoestrogens, corrosion inhibitor, perfluoroalkyl substances and pharmaceuticals. With this aim, four different sample preservation modes were tested: (i) in the raw seawater at room temperature, (ii) kept in a solid phase extraction cartridge of a mixture of Bond Elute Plexa (reverse phase) and Strata X-AW (weak anion exchange phase) sorbents at -20 °C, (iii) pre-concentrated in a polyethersulfone (PES) hollow fibres stored at -20 °C and (iv) in a methanol extract stored at -20 °C. The concentration of the target analytes (spiked at -240 ng/L) in the preserved modes were measured at six different times (0, 3, 10, 17, 24 and 31 days) during one month storage. In addition to this, the integrity of the supporting polymeric phases (PES, Plexa and Strata X-AW) was also studied by Raman spectroscopy, optical microscopy, and differential scanning calorimetric and thermogravimetric analysis.

As expected, different stability profiles were obtained: raw seawater samples showed the lowest stability (losses between 21-99 %), in SPE cartridges the average loss was 7 % and in the case of PES tubes losses up to 58 % were observed for acesulfame, caffeine, genistein, genistin, norfloxacin, OBT, PFBS, sulfadiazine and sulfamethoxazole. Though the complementary analyses of the supporting polymers showed that lowest integrity of the hollow fibre extracts may be related to the wettability of the PES as it was observed through the thermogravimetric analysis.

Acknowledgements

This work was financially supported by the Ministry of Economy and Competitiveness and the European Regional Development Fund (ERDF) through the project CTM2014-56628-C3-1-R and by the Basque Government through the project IT-742-13. L. Mijangos and H. Ziarrusta are grateful to the Basque Government and to the Spanish Ministry for their pre-doctoral fellowships.

Study and conservation of an iron spur recovered from a coastal medieval necropolis (Ereñozar Castle, Bizkaia)

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KEY WORDS: Archaeological irons, molecular mapping, Structural and Chemical Analyzer (SCA), akaganeite,

The present work, made in collaboration with the Arkeologi Museoa / Archaeological Museum of Bizkaia, focuses on the study of a medieval metallic spur excavated from the archaeological site of Ereñozar (Bizkaia). In order to identify both, original and decayed materials, an analytical protocol divided into three distinct phases was applied.

As a first step, the molecular and elemental characterization of the object was performed in-situ by using portable and non-destructive systems. The results obtained through the use of the X-ray fluorescence (XRF) technique helps to understand that the iron matrix of the spur was decorated by a metallic coat composed of gold, silver and mercury. On the other hand, the molecular analysis performed by Raman spectroscopy allowed identifying the presence of four iron corrosion compounds: goethite, magnetite, lepidocrocite and akaganeite.

The identification of the corrosion products lining an archeometallurgical artefact is very important, since each of them can affect its conservation in a very different way. On the one hand, goethite and magnetite are highly stable compounds that create compact corrosion layers that help to protect the object core from further degradations. On the other hand, lepidocrocite and akaganeite are extremely reactive phases facilitating cracks and loss of material phenomena.

Then, cross sections of several corrosion samples were prepared with the aim of carry out more detailed analysis with the help of laboratory systems. The elemental distribution maps made by using a scanning electron microscope (SEM) emphasized that Au, Ag and Hg are not part of the same decoration layer. In fact a gold coat applied by mercury gilding technique overlies a pure silver decoration applied in an earlier phase.

In addition, molecular maps carried out by inVia confocal Raman system allowed characterizing the stratigraphic succession of the iron corrosion phases. Thanks to this analysis it was possible to observe that the development of the most reactive phases was concentrated in the areas with the highest concentration of chloride ions.

In the third phase, the inVia confocal Raman was coupled to the SEM by using the SCA (Structural Chemical Analyzer) interface. This tool, developed by Ranishaw, allowed performing molecular analysis of samples taking advantage of the high resolution of the electron microscope. In this way, several degradation forms of micrometer scale were observed. Among them, the detection of silver chloride helped to demonstrate that the highly degraded aspect of the silver layer was due to the development of Cl-containing phases.

In conclusion, It is important to underline that the obtained results represented a very valuable resource for conservators, helping them on choosing the most appropriate conservation protocol. In this way, the important role that scientific research plays in the cultural heritage conservation field has been further demonstrated.

Chiral Brønsted Acid Catalyzed Enantioselective α -Amidoalkylation Reactions: A Joint Experimental and Computational Study

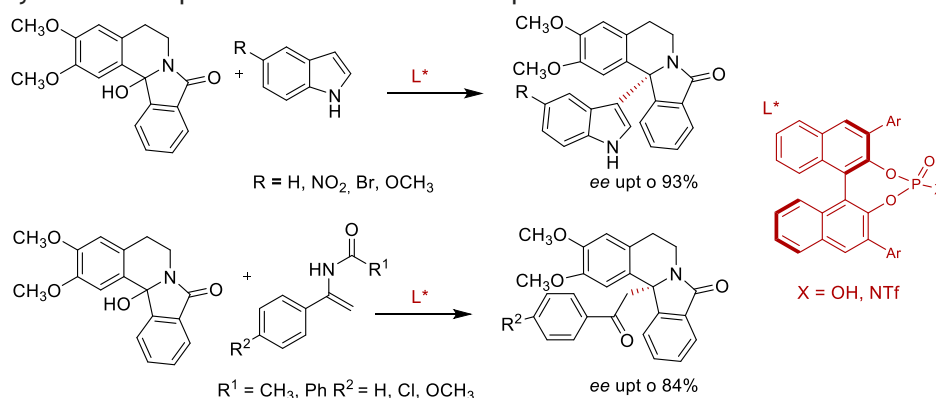
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KEY WORDS: asymmetric synthesis, organocatalysis, chemoinformatics

The α -amidoalkylation reaction is one of the most attractive methods for C–C bond formation in heterocyclic chemistry and has found widespread application in natural products synthesis. In the context, we have developed two strategies, aromatic metalation / intermolecular α -amidoalkylation and nucleophilic addition of organolithiums / intramolecular α -amidoalkylation sequences, for the diastereoselective preparation of fused indolizidines and quinolizidines, either using substrates from the chiral pool or chiral auxiliaries.¹ Now we are involved in the study of the enantioselective variant of both types of inter- and intramolecular α -amidoalkylations via cyclic and bicyclic N-acyliminium ions using chiral Brønsted acids (mainly BINOL derived phosphoric acids and *N*-triflyl phosphoramides) and H bond donors (mainly thioureas) as organocatalysts.²

Thus, we have investigated the enantioselective intermolecular α -amidoalkylation reaction of bicyclic hydroxylactams derived from *N*-phenethylphthalimides using a variety of π -nucleophiles as indoles (up to 93% ee)² or enamides (up to 83% ee). However, as the results have not been completely satisfactory and, in some cases, difficult to rationalize, we decided to use computational multi-target QSRR (quantitative structure-reactivity relationship) methods³ to predict the enantioselectivity in this type of intermolecular α -amidoalkylation reactions using enamides as nucleophiles. The main goal is to provide a simple and reliable tool to predict the enantioselectivity in this process, developing models to rationalize the stereoselectivity and thus orient the choice of the catalyst and/or experimental conditions to improve the results.



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Unravelling the growth of supramolecular metal-organic frameworks (SMOFs) based on metal nucleobases entities

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KEY WORDS: SMOF, nucleobases, porosity, adsorption, magnetism.

The present work provides a novel synthesis approach to obtain a new type of porous material based on supramolecular interactions called SMOF (supramolecular metal-organic frameworks). These compounds are related to the well-known MOF (metal-organic frameworks) but instead of being sustained by coordinate bonds, the metal-organic structural units are linked by hydrogen bond pairing interactions and/or π - π interactions in such a way that the growth of 3D supramolecular network renders an open-structure. Our research work has enabled us to establish the principles to successfully design and synthesise SMOFs, which are summarised in the following key factors:

1. The use of rigid metal-organic entities as building units, in which the rigidity is accomplished by at least the establishment of two coordination bonds or one coordination bond and a hydrogen-bond intramolecular bond.
2. The establishment of predictable and rigid synthons between the building units like double or triple complementary hydrogen bonding interactions.
3. The non-coplanarity of functional groups involved in the predictable synthons with the purpose of obtaining three-dimensional extended porous supramolecular assemblies.

In order to fulfil the above mentioned prerequisites, we have selected metal-nucleobase entities as building units due to the ability of these N-ligands to establish multiple coordination bonds with metal ions and base pairing interactions. The suitability of this synthetic strategy supported by several SMOFs, in which the structure design factors and synthesis conditions are considered.

Moreover, the SMOFs are exhaustively characterized by thermal analysis, adsorption and magnetic measurements. Thermal analysis reveals that the stability of SMOFs is similar to the conventional MOFs. Regarding the adsorption properties all the present materials are microporous with computed specific surface areas 800 - 3600 m²/g. It must be pointed out, that some of the studied examples are highly selective toward carbon dioxide adsorption when compared to dinitrogen, methane or hydrogen adsorption.

Finally, among the herein presented SMOFs, there is one consisting of heptanuclear Cu(II) wheel entities which have interesting magnetic properties. The inspection magnetic susceptibility curves indicates that the central copper(II) center is antiferromagnetically coupled to external copper(II) centers which are ferromagnetically coupled among them leading to a $S = 5/2$ ground state.

Magnetic Nanoparticles for Biomedical Applications

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KEY WORDS: Nanoparticles, magnetite, functionalization, magnetic hyperthermia, anti-tumour therapy.

The size confinement to nanometer scale in magnetic materials changes the properties from those of the bulk ferro and ferrimagnetic counterparts, the remainder magnetization disappears keeping the magnetic moment. These properties are interesting for some biomedical applications, such as drug delivery, magnetic resonance imaging or magnetic hyperthermia. The later one is based on the heating ability of magnetic nanoparticles (MNPs) under an alternating magnetic field and represents a therapeutic concept to cancer treatment, as cancer cells are more sensitive than healthy ones to temperatures higher than 41°C. The most usual materials for such applications are the superparamagnetic iron oxide (SPIO) compounds such as magnetite or ferrites which have a high magnetization and required compatibility with the biological medium.

A huge number of works have already reported great successes in producing magnetite nanoparticles by chemical methods in the most diverse morphologies, sizes and surface properties. Despite this, the use of these systems for clinical treatments is not as developed. Additionally, the role of the particle size and its functionalization on the performance of certain biomedical applications, in particular hyperthermia, remains obscure from the experimental point of view. Furthermore, these systems require having a high biocompatibility difficult to obtain.

In this sense, this group has optimized the preparation of Fe₃O₄ and Fe_{3-x}MO₄ (M = Zn, Mn) nanoparticles by a modified solution-phase thermal decomposition of metal precursors with 1,2-hexadecanediol as dispersant, benzyl ether as solvent and oleic acid and oleylamine as coating. The innovation is the utilization of the seeded-growth method based on successive additions of reagents over previously synthesized magnetic nanoparticles. One of the major aims of this work is to show how the refinement of this synthetic approach can be actually used to tune the size of the nanoparticles in the 5 - 25 nm range, producing nanoparticles with a very high crystallinity, small surface effects and magnetization values close to bulk magnetite. Moreover, it's possible to stabilize the nanoparticles in physiological medium by coating with amphiphilic polymers as PMAO and deliver them to a certain tumoral tissue by means of a specific bioconjugation with peptidic molecules of the RGD type. The chemical, structural, morphological and spectroscopic characterization of the particles has been performed by thermogravimetric analysis, X-ray diffraction (XRD), Dynamic Light Scattering (DLS) and Transmission Electron Microscopy (TEM). To study the magnetic behavior of the samples, magnetization measurements were carried out in function of magnetic field and temperature, as well as Electron Magnetic Resonance Spectroscopy (EMR) measurements. EMR spectroscopy has been shown as a powerful tool to evaluate magnetic size distributions of MNPs, allowing also an estimation of the heating power of the samples.

The final task of this project is to apply these nanoparticles for the destruction of cancerous tissues *in vivo* assays. So, magnetic fluids have been administrated to rats with hepatic tumour implants, but instead of injecting the fluids of NPs directly into liver tumours, intravascular administration of MNPs in animals have been performed. Afterwards the animals have been exposed to an alternating magnetic field, in order to achieve magnetic hyperthermia. Nowadays we are studying the evolution in an *in vivo* model and analyzing the reduction in tumour viability.

Cathodic composites for Li-ion and Na-ion batteries

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KEY WORDS: Li-ion and Na ion batteries, electrochemistry, spinel, lithium manganese phosphate, sodium vanadium fluorophosphates.

The search for commercially viable Li-ion and Na-ion batteries demands the discovery and optimization of new electrode materials and electrolytes in order to obtain more economic, safer and longer-life batteries.

Actually the research of cathodic materials is moving towards the development of electrode materials based on the abundance and availability of the relevant chemicals. Regarding to lithium ion batteries, lithium manganese oxide spinel is especially interesting for use in hybrid electric vehicles and electric vehicles due to its low cost and high safety. However, the main problem for application is the capacity fading caused by the instability of Mn(III). In order to improve that factor, in this report we investigate the effect of substitution of a small quantity of Mn by p-block elements such as Ga³⁺ or Si⁴⁺. The Li(Mn,M)₂O₄ (M = Ga³⁺, Si⁴⁺) phases have been synthesized by the freeze-drying method and calcinated at 700°C [1]. Another interesting material is the LiMnPO₄ olivine compound. Unfortunately, the electronic and ionic conductivity of LiMnPO₄ is insufficient for good electrochemical performance. The most widespread solutions are reduction of the particle size to nanometric scale, surface coating by an electronic conductor, or structural substitution by small amounts of metallic cations. In this work, nanosizing, carbon coating, and substitution have been combined in order to produce new and better-performing cathode materials based on Li(Mn_{0.8}Fe_{0.1}M_{0.1})PO₄/C (M = Fe, Co, Ni, Cu) composites [2].

On the other hand, the low cost, high abundance and ease of acquisition of sodium minerals promote interest in sodium-based electrochemical systems, especially for stationary energy storage devices. However, significant challenges such as energy density and long term stability must be addressed.

In general, Na₃V₂O_{2x}(PO₄)₂F_{3-2x} sodium-vanadium fluorophosphates are good cathodic materials for Na-ion batteries due to their high reaction voltages (at 3.6 and 4.1 V vs. Na/Na⁺) and their good specific capacity values in sodium half-cells (theoretical specific capacity of about 130 mAh/g) which leads to high energy density compounds (ca. 500 Wh/kg)[3].

In this study, two sodium-vanadium fluorophosphate materials were prepared by two different hydrothermal synthesis:

- A mixed valence V³⁺/V⁴⁺ composite material belonging to the Na₃V₂O_{2x}(PO₄)₂F_{3-2x}/C family where 0<x<1.
- Na₃V₂O₂(PO₄)₂F phase (x = 1) where vanadium oxidation state is V⁴⁺.

In all the cases structural characterization of the composites was performed by powder X-ray diffraction (XRD). Magnetic susceptibility measurements and EPR (Electron Paramagnetic Resonance) polycrystalline spectra were necessary for the determination of the oxidation state of the vanadium. The morphology of the materials was analyzed by Scanning and Transmission Electron Microscopy (SEM/TEM) and the electrochemical measurements were conducted using coin-cell and Swagelok-type cells *versus* a metallic lithium or sodium anode.

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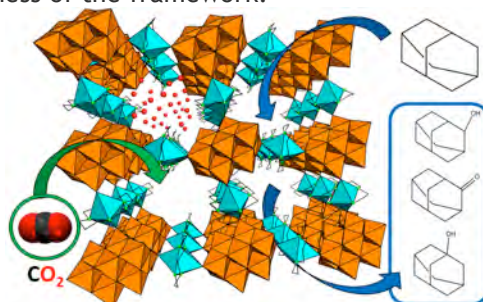
Multifunctional Nature of Polyoxometalate-based Open Hybrid Frameworks

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KEY WORDS: POMOFs, porosity, gas adsorption, heterogeneous catalysis.

Porous crystalline materials such as metal organic frameworks (MOFs) have attracted great attention due to their wide range of relevant applications. These materials are constructed by coordination of metal ions or metal-containing units (nodes) to organic bridging ligands (linkers) to form open crystalline frameworks with permanent porosity. This feature qualifies them as suitable candidates for gas storage and separation, ion exchange, host-guest chemistry, magnetism, biomedicine and catalysis. However, the synthesis of MOFs usually requires harsh conditions (e.g. high temperature or pressure, prolonged reaction times, harmful solvents, etc.), and removal of guest molecules from their cavities often leads to the collapse of the porous structure when flexible linkers are used. In this context, the incorporation of rigid and voluminous species such as metal clusters could increase the overall mechanical and thermal stability of the framework. Among metal clusters, polyoxometalates (POMs), which are a family of anionic metal oxo clusters with large topological diversity and intrinsic multifunctional nature, have been identified as excellent building blocks for the construction of such robust, high-dimensional open structures. Moreover, compared to MOFs, the synthetic requirements for the assembly of POM-based extended structures usually involve milder conditions, aqueous reaction media and easier counterion exchange. Nowadays, POM-based crystalline solids with permanent porosity are of great interest because inherent features of POMs such as reversible redox properties or high catalytic site density can be combined with the characteristics derived from open-framework structures. In our last work,¹ the first POMOF-like hybrid compound with supramolecular microporous open-framework based on decavanadate clusters, namely $[\text{Cu}(\text{cyclam})][\{\text{Cu}(\text{cyclam})\}_2(\text{V}_{10}\text{O}_{28})] \cdot 10\text{H}_2\text{O}$ (**1**), has been synthesized and fully characterized. The supramolecular architecture contains covalent decavanadate/ $\{\text{Cu}(\text{cyclam})\}$ grids with square-like voids the stacking of which is driven by a massive network of intermolecular N-H \cdots O and C-H \cdots O interactions established with interlamellar cementing complexes. The structure is able to remain virtually unaltered upon thermal evacuation of guest solvent molecules located in the system of parallel channels generated by the stacking of the hybrid layers, as evidenced by a single crystal X-ray diffraction studies on the anhydrous **1a** derivative. The permanent microporous nature of **1** results in functional properties such as selective adsorption of CO_2 gas over N_2 and remarkable catalytic activity toward the oxidation of the highly-stable organic substrate adamantane in heterogeneous phase. To our knowledge, this is the first decavanadate-based hybrid compound that shows both CO_2 sorption capability and catalytic activity in the oxidation of cycloalkanes owing to its microporous nature, accessibility of channels and robustness of the framework.



¹Jagoba Martín-Caballero, Ana San José Wéry, Santiago Reinoso, Beñat Artetxe, Leire San Felices, Bouchra El Bakkali, Guido Trautwein, Juan Alcañiz-Monge, José Luis Vilas and Juan M. Gutiérrez-Zorrilla *Inorg. Chem.* **2016**, *55*, 4970–4979.

Defect structure of battery materials with FAULTS program

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KEY WORDS: FAULTS, X-ray refinement, stacking faults, battery lithium-ion, lithium rich.

X-ray and neutron powder diffraction (XRD or NPD) are commonly used techniques to elucidate crystal structures. Once the structural model has been built, it is usually refined by means of the Rietveld method so as to obtain accurate structural information. However, the Rietveld method faces several limitations in the case of crystalline materials with extended defects such as stacking faults, since these are poorly described with an average unit cell. The FAULTS program [1], now integrated in FullProf suite, is able to calculate diffraction intensities from defective crystals. It is based on the simulation program DIFFaX [2,3] which has been extended to enable the refinement of experimental XRD and NPD patterns of faulted crystal systems. As in DIFFaX, the structure is described as a stack of layers to form the 3D structure, which enables us to include this kind of defects in the structural model. Using this tool it is then possible to extract quantitative information regarding the type and amount of stacking faults, and to correlate these to material's properties. In figure 1 the difference between a Rietveld and a FAULTS refinement is shown in the case of Li_2MnO_3 , a promising Li-ion battery high energy density cathode material. This material usually crystallizes with stacking faults which have hampered to date an accurate description of its real structure. We will show how the FAULTS program is able to do so and how the FAULTS program can be applied to precisely describe the structure of different types of functional materials with planar defects.

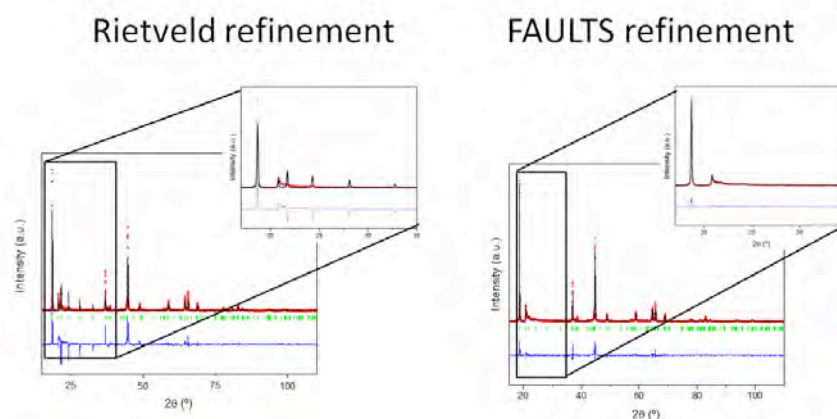


Figure 1. Rietveld (left) and FAULTS (right) refinement of Li_2MnO_3 defective structure.

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Study of organocatalytic normal electron demand [5+2] cycloadditions

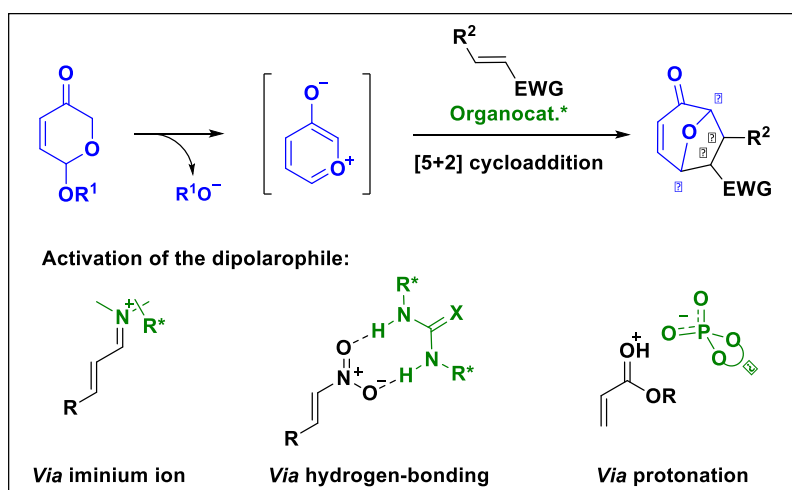
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KEY WORDS: asymmetric catalysis, cycloaddition, organocatalysis, iminium ion, hydrogen-bonding catalysis, Brønsted acids.

The stereocontrolled construction of chiral carbocycles and heterocycles is an important field of research in modern organic synthesis, and asymmetric organocatalysis has been efficiently employed to achieve that stereoselectivity.¹ In this sense, [5+2] cycloaddition reactions constitute an effective methodology to get seven-membered ring structures, including the privileged bicyclic scaffold 8-oxabicyclo[3.2.1]octane, which is present in numerous bioactive natural products.²

Recently, our research group has developed an organocatalytic enantioselective version of the target reaction under dienamine activation, which allows access to the desired products with good yield and high selectivity.³ With these precedents in mind, we have studied the viability of organocatalytic [5+2] cycloaddition reactions between oxidopyrylium ylides as dipoles and electron deficient olefins as dipolarophiles to build up products containing the 8-oxabicyclo[3.2.1]octane in a regio-, diastereo- and enantioselective manner. For this purpose, different activation modes of the dipolarophile have been used, such as activation of aldehydes via iminium formation, of nitroolefins via hydrogen-bonding catalysis and of acrylates by employing Brønsted acids, obtaining in all cases the cycloaddition products with different yields, regio- and diastereoselectivities, although with poor enantioselectivity.



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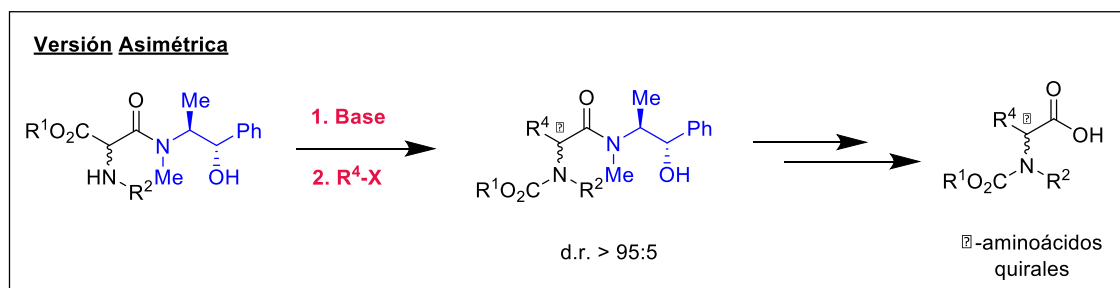
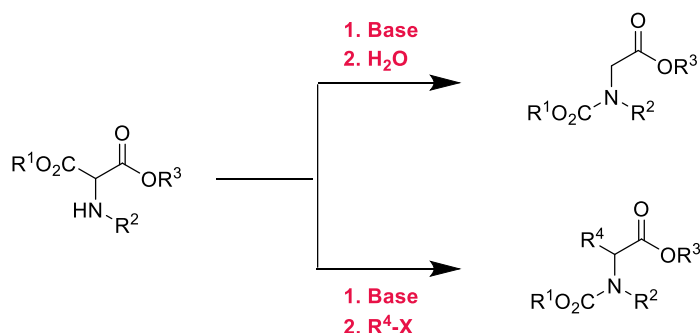
Asymmetric Version of the base promoted C→N Transfer Reaction using Chiral Auxiliaries

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KEY WORDS: rearrangement reaction. pseudoephedrine, tandem reaction

Decarboxylative protonation of substituted aminomalonates and derivatives is a synthetically convenient and straightforward route to synthesize a variety of unnatural α -amino acids, biologically important organic compounds which are used in chiral pool synthesis as enantiomerically pure building blocks. Recently, our group has established a good approach to this decarboxylative protonation process, developing a novel base-promoted rearrangement reaction that converts N-substituted α -aminomalonates into N-alkoxycarbonyl α -amino acid derivatives under mild conditions. Moreover, it should be emphasized that this methodology provides a wide range of α -alkylated products in good yields when the enolate intermediate is trapped by alkylation in a tandem sequence.

Herein, we present the asymmetric version of this protocol in which (S,S)-pseudoephedrine amides derived from malonic acids have been studied as decarboxylative reactant for further alkylation with an external electrophile obtaining a wide range of α -alkylated products in good yields.



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Cross-coupling reactions in water catalyzed by a palladium phosphinite complex

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KEY WORDS: cross-coupling, palladium, water.

Since the birth of “Green Chemistry”, scientific community has striven for the development of cleaner and more environmentally friendly synthetic routes. In this sense, the use of catalysts has contributed in an important way reducing reaction times and thus the inherent energy cost. On the other hand, new and more versatile catalytic systems are discovered every day. Among these catalytic systems we can find pincer-type complexes, metallacycles bearing a tridentate ligand that have demonstrated a higher thermal stability as well as a remarkable catalytic activity in a plethora of synthetic reactions such as Michael additions, allylation reactions, alkane metathesis, transfer hydrogenation, cross-coupling reactions etc. The latter have proved to be an advantageous tool for the construction of C-C bonds due to their ability to build complex scaffolds in both intramolecular and intermolecular fashion.

Herein, the synthesis of a new non-symmetric pincer type catalyst is presented. This complex was prepared in two steps, starting from the commercially available and cheap 1*H*-pyrazole and 3-bromophenol. An initial *N*-arylation followed by a tandem phosphorylation/palladation provided the desired product in a good overall yield.⁴

After full characterization, the new phosphinite-bearing palladacycle was further assayed in Suzuki-Miyaura cross-coupling reactions. To our delight, water turned out to be an optimal solvent for such transformations, which were carried out using minimal catalyst amounts (10^{-2} - 10^{-6} mol%).

Use of magnetically active iron compounds in a tandem reaction involving alkynoic acids

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KEY WORDS: iron catalysts, cascade reactions, magnetic materials.

The development of more sustainable and efficient methods is one of the key goals in chemistry research. In this regard, catalysis has proved to be crucial in the development of new compounds. During the last decades, many transition metal catalysts, especially those based on “precious” metals such as palladium, rhodium, iridium or ruthenium, have proven to be effective for many applications achieving an excellent level of activity and selectivity. However, the limited availability of these metals, their high price and toxicity have led to the search for cheaper and environmentally respectful alternatives that minimize the generation of toxic substances. In this context, iron based catalysts offer significant advantages over precious metals, and in recent years an increasing number of synthetic applications have been found for iron catalysts.

Following our research on cascade reactions promoted by iron catalysts, we have developed an advantageous procedure for the use of magnetically active iron species (Fe(0) and magnetite) in the one-pot preparation of polyheterocyclic systems from alkynoic acids. Magnetic decantation provided a protocol for the separation of reaction products from catalysts and their recycling.

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Advances in the understanding of catalyst deactivation in the steam reforming of bio-oil

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KEY WORDS: steam reforming, deactivation, coke deposition, bio-oil.

INTRODUCTION AND OBJECTIVES. The depletion and environmental pollution from fossil fuels call for using new energy resources. Hydrogen has a very high energy density (~121 MJ/kg) and provides a clean energy source for the production of chemicals and is an alternative to conventional automotive fuels. Catalytic steam reforming of bio-oil (produced from the pyrolysis of lignocellulose) is considered a viable and promising route for hydrogen production. The process can be materialized with delocalized pyrolysis units, transport of the produced bio-oil to bio-refineries, and subsequent steam reforming. Nickel-based catalysts have been widely used in the literature for steam reforming of bio-oil, due to the high C-C bond-breaking activity and the relatively low cost. Although high conversion and H₂ yields can be achieved, the catalyst undergoes a rapid and severe deactivation, both by sintering and, more notoriously, coke deposition. The complexity and heterogeneity of the composition of bio-oil (acids, ketones, alcohols, phenols and guaiacols, among others) makes it difficult to establish coke formation mechanisms during bio-oil steam reforming, which is of the utmost relevance in order to inhibit its formation routes. Consequently, the entire process would benefit by identifying the main deactivation causes. This work aims at progressing in the understanding of catalyst deactivation during the steam reforming of bio-oil, as well as establishing a correlation between several influential variables during its deactivation.

EXPERIMENTAL. The Ni/La₂O₃- α Al₂O₃ catalyst contains 10 wt% Ni and 9 wt% La₂O₃, prepared by incipient wetness impregnation method. Steam reforming of bio-oil took place in a catalytic fluidized bed reactor: temperature, $T=550-700$ °C; time on stream, 4 h; fed steam to carbon ratio, $S/C=1.5-6$; space time, $0.19 \text{ g}_{\text{cat}} \text{ h g}_{\text{bio-oil}}^{-1}$. The composition of the reaction medium was determined by GC/MS analysis. The morphology, content and composition of the catalyst and coke were studied by several characterization techniques displayed below.

RESULTS AND DISCUSSION. Firstly, an increase in T and S/C contribute to a higher catalyst activity, as decomposition and polymerization of coke precursors are inhibited, and both steam reforming and gasification of coke precursors are favored, as well as the gasification of coke in case of having been formed. An study of the coke nature (TG-TPO thermogravimetry, SEM & TEM microscopy), allows the identification of two types of coke within its structure: (i) a less-developed coke mainly deposited at a lower T , which encapsulates Ni particles, and (ii) a coke with a higher structuring grade, mainly grown in filaments at a higher T . T has showed to be the most influential factor both in the composition of the reaction medium (GC/MS) and the coke (FTIR). Furthermore, an interesting correlation between these two compositions was observed. S/C ratio is the most influential factor in the deposited coke content (TG-TPO): lower coke deposition at higher steam proportion in the medium. On the other hand, temperature is the most influential factor in the coke structure (XPS, FTIR, Raman, FTIR-TPO): more disordered, aliphatic and oxygenated at lower T , and more developed and aromatic at higher T . Coke nature has showed to be a determining factor for a higher desactivation degree, whereas higher coke content may be influential but not determining. Thus, the encapsulating nature of coke at lower T is pointed as the main catalyst deactivation cause, covering the active sites and catalyst surface, while at higher T , the developed filaments involve a significantly lower deactivation, as surface porosity is increased and Ni sites are more accesible. Ni particle sintering was observed at high T (700 °C) by XRD and TEM; however, as reforming and gasification reactions are favored, a lower deactivation is observed compared to 550 °C, where no Ni sintering was observed.

Towards the implementation of fine particle treatment processes in conical spouted bed

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KEY WORDS: Fine particle, conical spouted bed, drying.

INTRODUCTION AND OBJECTIVES

This research is framed in the joint project of Catalytic Process & Waste Valorization Research group, (University of the Basque Country, UPV/EHU) and Novattia Desarrollos Ltd., technology Development Company, with the objective of designing a new dryer for fine and ultrafine sands based on spouted bed technology.

It is known that the spouted bed is a valid technology for a variety of processes such as drying, coating, blending and encapsulation of particles of group B or D of Geldart [1], being this last group of particles the most widely developed. However, the processing of smaller particles with a broad size distribution is an underdeveloped area, so the advances in this field could open new ways of research and even give rise to new design projects of equipments for industrial processes. Kmiec and Szafran [2] did a good review of conical spouted bed applications, emphasizing the use of a draft-tube to stabilize the spout regime of small particles ($d_p < 1$ mm). Moreover, working also with fine particles (sands), Altzibar et al. [3] found that the use of a porous draft tube allows for gas percolation to the annular zone. In this paper, a conical spouted bed provided with a draft tube and confinement system has been studied to verify its potential application in the drying of fine and ultra-particles and with a broad size distribution.

METHODOLOGY

The materials used in the study are: (1) fine sand with a wide particle size distribution between 0 and 800 μm which a 90% of particles of Geldart's group B AND a 10% of group A and (2) ultrafine sand with a narrower particle size distribution between 0 and 120 μm but with 96% of group A and a 4% of group B.

The contactor consists in a PMMA vessel with a height of 1.16 m, 0.36 m of diameter of the upper cylindrical section and 0.068 m of base diameter and 36° of cone angle. The contactor has the possibility to be used with different gas inlet diameters and allows including draft-tubes at its inlet. In the study 0.04 and 0.05 m of inlet diameter have been used, together with five non porous and nine open-sided draft-tubes. Moreover, the contactor has a confinement system that consists in a PMMA pipe of 0.2 m diameter and 0.6 m length, having the upper end closed. Along the research the contactor has scaled up to a stainless steel vessel to realize batch and continuous drying and several improvements have been added to make the experimentation easier and more precise or to improve the drying efficiency. All equipment is coupled to an air blower, and particles dragged by the air out of the contactor are retained with a bag filter.

MAIN CONCLUSIONS AND ACHIEVEMENTS

- It has been achieved fluidize materials until now unused in this kind of technology.
- Improvements as the confinement system have been included that benefit both fluid-dynamics and the drying process.
- Encouraging start of the continuous study with very high energy efficiency.

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Kinetic and thermal analysis of the dehydration process NFMD of encapsulated probiotic material

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KEY WORDS: microencapsulation, drying, microwave, food additives.

In this work, a mathematical model for the description of the drying process named Near Fluidizing Microwave Drying (NFMD) process is carried out on the basis of the mass and energy balances. The model is applied to the experimental results of the NFMD for the dehydration of two different encapsulated probiotics materials: *Saccharomyces Cerevisiae* and *Bifidobacterium bifidum*.

The mathematical model, implemented in FlexPDE®, has been elaborated to fit the experimental data. The kinetics adjustment has been developed through parameters: b , regarding boundary moisture values and D representing the effective diffusivity. These values change for the different thermal levels applied. The shrinkage has been contemplated by the density of the particles as a function of time. From the thermal profiles, some parameters like the electric field and the convection coefficient were evaluated for the energy consumption analysis. Kinetic and energy parameters are required to analyze the effect of the operational variables: microwave power and air temperature and their effects on drying rate and efficiency of drying.

The mathematical model applied describes adequately the drying kinetic and the thermal profiles in a NFMD process, being necessary to consider three phases in the drying process. Coefficient b , regarding moisture boundary conditions, and the effective diffusivity D , were both needed to fit the mass loss drying kinetics. While b value remains constant during the process, D values change in each phases. The diffusivity during the phase II presents the highest value coincident with the maximum drying rate. Coefficient D was found in general to be tenfold lower than in phase I, probably due to the greater participation of the vapour diffusion mechanism.

Besides, NFMD process was evaluated with and without volume shrinkage consideration. Diffusivity decreases when volume shrinkage is considered, with Experiments 4 and 5 of BB12® presenting the largest differences. The major effect of the volume shrinkage seems to be related to the experiments with the highest diffusivity values while little significance was found in the experiment of lower drying rate.

Other aspects analysed were the heat parameters: convective coefficient, h , and electric field E that serves to estimate the heat absorbed by the product and subsequent energy consumption. The low thermal level and a medium gradient imply a reduction of energy consumption, corresponding to most efficient strategies associated to the most favourable drying kinetics and energy consumption. However, the definitive selection must be carried out by considering additionally the quality and viability of the product.

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Power-to-gas: CO₂ methanation with renewable hydrogen

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KEY WORDS: Climate Change, renewable energy, CO₂ recycling, catalytic CO₂ hydrogenation into CH₄

The excessive emission of anthropogenic greenhouse gases (especially carbon dioxide) derived from the production of energy by combustion of fossil fuel carries global warming and severe climate change that threatens the well-being of society. In recent decades, many efforts have been made to develop efficient renewable energy sources that reduce the amount of CO₂ emitted. The major drawback of renewable energy is its intermittency; wind and solar energy are fluctuating and have to be balanced for electric grid stability purposes. Consequently, large capacity electricity storage is required, as well as, reserve production capacity.

Power-to-gas (PtG) process is considered as a possible and interesting solution to integrate renewable resources, such as wind and solar energy, into the current energy mix efficiently. The PtG process links the power grid with the gas grid by converting surplus power into a grid compatible gas via a two step process: H₂ production by water electrolysis and H₂ catalytic conversion with an external CO₂ source to CH₄ via methanation. The resulting CH₄, known as synthetic natural gas (SNG), can be injected into the existing gas distribution grid, used as motor fuel, or it can easily be employed in other well established natural gas facilities.

In recent years, several studies have been carried out on supported catalyst formulations for CO₂ methanation or synthetic natural gas production (SNG). These formulations mainly consists of group VIII B metals (Fe, Ru, Co, Rh, Ir, Ni, Pd, Pt) supported on various oxides (e. g., SiO₂, TiO₂, Al₂O₃, ZrO₂, CeO₂ and Ce-Zr mixed oxides). Metals that have provided greater activity in CO₂ hydrogenation have been Ru and Rh, although Ni has covered higher number of published works due to its good relationship between activity and price. The main reported problem of Ni-based catalysts seems to be deactivation at low temperature due to the interaction of the metal particles with CO and the formation of mobile nickel carbonyls that lead to the metal sintering. In order to avoid sintering and enhance catalytic activity of Ni-based catalysts, various strategies have been tried, such as adding promoters to the catalyst systems, altering the type of supports and preparation methods.

Another important issue concerning the activity, selectivity and stability of catalysts is the nature of the support. In fact, the different interactions that can be established between the metal and the support and the presence of different basic sites in the support could influence the catalytic behaviour. Catalysts with γ -Al₂O₃ and Ce-Zr mixed oxides as supports have presented the most interesting properties for the methanation reaction. The good performance of catalysts containing CeO₂-Zr₂O₃ is attributed to its higher ability to adsorb CO₂ molecules in weak and medium basic sites, to reduce them into CO and to convert CO into CH₄.

Our research is focused on the design of Dual Function Materials (DFM) able to capture CO₂ and simultaneously convert it into CH₄. DFM material consists of a supported catalyst that contains a sorbent and a catalyst component. We propose zeolite as a possible support, since it has been scarcely studied. This kind of support provides a high surface area in which active site (Ni in that case) can be well dispersed. Zeolite based catalysts show synergetic interactions among the metal site and the support which provide remarkable activity ($X_{\text{CO}_2} \approx 70\%$) and selectivity. It has to be pointed out that zeolite support can hardly adsorb CO₂ and hence, requires the addition of sorbents such as CaO or MgO. The basicity of the zeolite can easily be modulated by adding alkali earth metals that provide new sites in which CO₂ molecule is activated.

Free Pt group metals catalysts based on modified perovskites for the NO_x removal from diesel engines exhaust gases

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KEY WORDS: Perovskites, NO_x, exhausts, diesel engines, Pt group, NSR, SCR.

The work summarized in this contribution is focused on the use of alternative catalysts to Pt group metals for cleaning gas effluents from diesel engines, mainly centered on those which are most difficult to eliminate.

Increased environmental awareness, legislative measures and public demand for environmental sustainability are leading to an increase in diesel engines in developed countries. The operation with higher air/fuel ratios results in a higher fuel efficiency and lower greenhouse gases emission. Nevertheless, NO_x are particularly difficult to remove from oxidizing exhausts such as those in diesel vehicles

Over the last years, the TQSA research group has focused its efforts on the development of catalytic systems for the two main technologies proposed for the removal of NO_x from exhaust gases released by diesel engines: NO_x storage and reduction (NSR) and NO_x selective catalytic reduction (SCR).

The former technology (NSR) requires a catalyst combining sites for NO_x adsorption and metallic sites able to favor oxidation and reduction reactions. A model NSR catalyst consists of platinum and barium supported on alumina. During normal operation, oxidizing exhaust gases containing NO_x pass through the catalytic bed. NO_x is adsorbed on the catalytic surface until saturation. Then, a reducing agent such as hydrogen is injected for a short time to the gases entering the catalytic bed, and adsorbed NO_x are desorbed and reduced preferentially to N₂. The latter technology (SCR) uses zeolitic structures interchanged with metals as catalysts. A model SCR catalyst consists of a Cu-zeolite. During operation, a small amount of NH₃ is mixed with the oxidizing exhaust gases entering the catalytic bed. NH₃ and NO_x are adsorbed on the catalytic surface, where they react to selectively produce N₂. Recently, both technologies have been combined in two catalytic beds arranged in series, NSR-SCR, which allows for virtually zero-emission exhausts.

Formulations developed up to date allow to achieve strict standards emission levels. However, high loads of Pt group metals (PGMs) with high price and poor thermal stability are required. For the total implementation of these technologies it is necessary to develop sustainable alternatives, with higher durability and more economical. Perovskites oxides described by general formula (ABO₃) have been proposed as an alternative which reduces costs comparing to PGMs catalysts in many heterogeneous catalysis processes. More than 90% of the metallic elements from the periodic table can enter the perovskite structure. That way, one of the main advantages of perovskite structures is the possibility to adopt a wide range of different compositions, changing either A or B cations or partially substituting each cation by others of the same or different valences to adjust their redox and surfaces properties.

Lanthanum based perovskites with Co or Mn as B cation have been synthesized for NSR process because of their high NO oxidation capacity. In order to improve redox and surfaces properties, some La is partially substituted by Sr. As a consequence; there is an improvement in NO to NO₂ oxidation and NO_x storage capacity, achieving higher or similar values to Pt-based catalysts. Recently, a combination of 30% of La_{0.7}Sr_{0.3}CoO₃ and 70% Pt-Ba/Al₂O₃ has shown similar activity to 100% Pt-based catalysts with lower cost and more durability.

Hydrogen production by catalytic aqueous phase reforming of biomass-derived oxygenated compounds

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KEY WORDS: Hydrogen production, fuel cell, aqueous phase reforming, biomass, glycerol, nickel catalysts, cobalt catalyst, metallic spinel, nanocasting.

TQSA group has focused the present research in the development of an active catalyst for obtaining hydrogen-rich streams from the aqueous phase reforming of oxygenated compounds. The synthesis of highly selective to H_2 , stable and cheaper than noble metal based catalysts is pursued. The main objective involves the valorization of glycerol, a byproduct of biodiesel production, which is a readily available feed.

The increasing economic development in the world has notably increased energy consumption, accelerating the depletion of fossil fuels. Additionally, there is a need for developing alternative energy supply strategies, which protect the environment and promote a transition from the actual fossil-fuel based economy to renewable energy based one. In this context, hydrogen is taking a relevant place as energy vector, promoting the development of fuel cell technology, with an added value of neutral net CO_2 balance whenever they are feed by hydrogen produced from biomass-derived oxygenated hydrocarbons.

The selective conversion of glycerol into hydrogen is addressed through the emerging aqueous phase reforming (APR) technology. It has notable advantages with respect to the gas phase steam reforming (SR), namely lower energy requirements, since evaporation of feed stock is not needed. Moreover, the production of high purity hydrogen is facilitated due to minor concentration of CO. The lower temperatures required favour Water Gas Shift (WGS) thermodynamics, which facilitates subsequent purification of the stream, prior to feeding to the fuel cell.

This project addresses the development of a cost-effective catalyst, active for C-C, O-H and C-H bond cleavage, whereas it preserves C-O bondings. Noble metal based catalysts are active, highly selective to H_2 and durable, but their cost is extremely high. Metals from group VIII, such as nickel and cobalt, are cheaper, but non conventional synthesis methodologies are necessary to obtain an attractive alternative to noble metal based catalysts. Among the catalysts developed for this purpose, metallic spinels (MA_2O_4 , $M=Ni, Co$) have been synthesized via coprecipitation and mesoporous siliceous templates (nanocasting route). These catalysts have been analysed by different characterization techniques in order to investigate their physicochemical properties.

The first screening of the synthesised catalysts has been performed by using glycerol/water synthetic mixtures, on a batch reactor. A Micro Gas Chromatograph (MicroGC) was used to analyze the composition of the gas-phase stream throughout the reaction. In addition, a Gas Chromatograph coupled to a Mass Detector (GC/MS) was used to analyse the trace liquid phase evolution. Obtained results will serve as the basis for the subsequent refinement and improvement of key catalytic properties of the materials in order to achieve high yield to gas and selectivity to H_2 , and control of carbonaceous deposits. A posterior screening will be carried out for extended periods of operation on a continuous micro-reactor which allows three-phase reaction.

ABSTRACTS

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BIOZIENTZIAK BIOCIENCIAS



Bacterial resistance to stress.

Survival strategies of *Vibrio* spp

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KEY WORDS: bacteria, *Vibrio*, adverse environments, resistance.

Microorganisms are exposed to periodic stresses that include changes in physicochemical parameters of the system as well as changes in their relationship with other organisms. Both abiotic and biotic factors drive the behavior of microbial populations. Nevertheless, bacteria can trigger a number of adaptation mechanisms to increase their capacity of persistence and survival in those changing environments.

Our group has previously studied the response of *Escherichia coli* (intestinal bacteria) to different abiotic stressors (starvation, sub-optimal temperature, luminous irradiation, etc.) as well as to the presence of natural microbial communities of aquatic systems (protozoa, autochthonous bacteria and bacteriophages). Our results indicate that abiotic factors promote physiological and molecular responses to ensure the persistence of a part of the population, the culturable fraction, at the expense of nonculturable cells generated by effect of stress. In these conditions, the formation of viable but nonculturable cells is subordinated to the boom and bust strategy. However, biotic factors can lead to the elimination of the bacterial population.

Subsequently, we have transferred this knowledge to the study of the behavior of *Vibrio harveyi* in aquatic environments. *V. harveyi* has a optimum growth temperature at 28°C but it can remain as nonculturable population in water maintained at 4°C, and recover the culturability again when temperature increases. *V. harveyi* also present a dual response to stress, however, the bust and boom process does not seem to be the main strategy to persist in the environment.

The ongoing increase in temperature of surface waters resulting from climate change has caused variations in the global incidence of diseases caused by *Vibrio*, reporting *Vibrio*-associated diseases in European countries where virulent variants were not habitual. Our group has initiated the study of the temporal distribution of *Vibrio* species on the coast of the Basque Country and we have isolated and identified *Vibrio* species present in the Biscay Coast to establish the seasonal dynamics for *Vibrio* spp. Moreover, we are studying the response to the biotic and abiotic parameters in several isolates in order to compare their survival strategies with those observed for *V. harveyi* ATCC.

Another field of interest of our group is the study of biological processes occurring during a wastewater treatment process by activated sludge. Wastewaters are the perfect vehicle for dissemination of several microorganisms. We study the importance of mechanisms implicated in the elimination of faecal bacteria during treatment: adhesion to flocs/sludge, elimination by grazing, parasitism, competition, etc.

Those questions have been analysed *via* traditional methods in microbiology, new molecular methodologies, the use of strains easily identifiable into complex matrices, etc. The techniques and methodologies used include: epifluorescence microscopy, fluorescence *in situ* hybridization, analysis of bacterial proteome, water quality analysis, test for disinfectants and other toxic compounds, etc.

Marine ecosystems: Insights from a microbial point of view

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KEY WORDS: marine ecosystem, bacterial diversity, ecological function

Variations in the structure of the microbial community in space and time are thought to play a major role in regulating the biogeochemical processes of aquatic systems. We are interested in the interrelationships among diversity and function of the prokaryotic community and the environment in both the open ocean and coastal waters.

OUR RESEARCH PROJECTS:

The Project “**Cambio. Bacterioplankton Diversity and function of the bacterioplankton in the Eastern Cantabrian Sea: Grazing and nutrients as drivers of the seasonal change**” (MICINN, CTM2010-19308/MAR) is focused on the:

- Identification of seasonal changes in relevant members of the community over a multi-year time scale and know the specific composition and diversity of the bacterioplanktonic community.
- Establish links between the taxonomic diversity and the physiological function of bacterioplankton and detection of possible drivers of the change of relevant members of the community.

The Project “**Circumnavigation Expedition Malaspina 2010; Global Change and Biodiversity Exploration of the Global Ocean**” (MICINN, CSD2008-00077) is an interdisciplinary project divided in 7 thematic blocks and 4 transversal blocks. The main objectives are:

- Assess the impact of global change on the ocean and explore the biodiversity and the functional role of the microorganisms in the biogeochemical transformations of organic matter, with special interest in the deep-sea.
- Specifically, our research group analyzes hydrolytic enzyme activities of the bacterioplankton in the global ocean: biogeographical variation, kinetic behavior, stability and relationship with the organic matter and the bacterial diversity.

Study of a marine bacteria culture collection using different techniques:

Molecular techniques for the identification, microscopic and macroscopic characterization (Gram staining and colony color and morphology observation), physiological characterization using selective culture medium, enzymatic production (milk agar (caseinase), cellulose agar (cellulase), starch agar (amylase) and DNA agar (DNase) and antimicrobial compound production.

Ocean Sampling Day (OSD)

The OSD is a global sampling around the world in June 21st of 2014 and 2015 with 191 sampling sites range from tropical waters to polar environments. It is a simultaneous, collaborative, global megasequencing campaign to analyze marine microbial community composition and functional traits on a single day. Together, they were collected 155 16S/18S rRNA amplicon data sets, 150 metagenomes, and a rich set of environmental metadata with a cooperation with the LifeWatch project, Pacific Bioscience and the Smithsonian Institute's Global Genome Initiative. Data analysis will target three main areas: biodiversity, gene functions, and ecological models.

Molecular Biology of Cancer

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KEY WORDS: Cancer, Cell Cycle, Cell Signaling, Ubiquitination, Gene knockout, Genomics, Proteomics.

The main feature that defines tumor processes is the alteration of cellular homeostasis. Deregulation of the cell cycle, abnormal intracellular signaling, and defects in protein posttranslational modifications are among the mechanisms that contribute to this alteration. The detailed characterization of these mechanisms, and how they contribute to the neoplastic transformation constitute the main objectives of our research group. Their elucidation could contribute to the search for new therapeutic strategies for cancer treatment.

Our research group is a multidisciplinary team whose components are specialized in the areas of genetics, molecular and cellular biology, proteomics, and bioinformatics. The group has been working for more than a decade in the field of molecular biology of cancer, considered to be a strategic research field by the Euskampus initiative of the UPV/EHU, because of its biomedical and social relevance. The research team has been recognized and funded by the Department of Education of the Basque Government as "Consolidated Group" continuously since 2001.

Research in Biomedicine has experienced an extraordinary revolution in recent years, with the development of technologies that allow the analysis of complete sets of genes and proteins in a particular cell or organism. This has led to the birth of the novel fields of Genomics and Proteomics. We are applying genomic and proteomic approaches, together with classical methods of genetic and biochemical analysis, to identify and characterize the proteins and pathways that play a key role in the control of cellular proliferation and cell fate, including the dysregulation that contributes to oncogenesis. Current areas of research in the laboratory focus on the following topics:

1. The Retinoblastoma/E2F regulatory pathway in cell cycle control. Aims:

- Transcriptional regulatory networks controlled by E2Fs
- Mechanisms by which E2Fs control DNA replication, DNA repair and cell cycle progression in vivo
- Mechanisms for cell fate determination mediated by E2Fs

2. Monomeric GTPases and their activity in intracellular signaling. Aims:

- Is the Rac1/Glycogen phosphorylase pathway conserved in other cell lineages and receptor systems?.
- Is the Rac1/Glycogen phosphorylase pathway involved in protein glycosylation (O-GlcAcylation)?.
- Is the Rac1/Glycogen phosphorylase pathway dysregulated in the rare disease Glycogenosis type V?

3: Ubiquitination and nucleocytoplasmic transport of proteins during tumor development. Aims:

- Novel substrates and functions of the USP1/UAF1 deubiquitinase complex
- Effect of cancer-related mutations of the USP1/UAF1 deubiquitinase complex
- Effect of cancer-related mutations of CRM1 in nuclear export receptor
- Therapeutic effect of CRM1 inhibitors in cancer

4: Development and application of proteomic technology. Aims:

- Identification of new effector molecules involved in transduction of the proliferative signals by label-free expression proteomics.
- Optimization of shotgun and targeted techniques for the identification and quantification of proteins by mass spectrometry.

Adaptation and resilience of plants to climate change

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KEY WORDS: Barley cultivars, climate change, conventional farming, CO₂ sinks, drought, elevated CO₂, legumes, organic farming, plant physiology, production, resilience.

Climate is a major influence factor affecting agricultural production, and any change on it can reduce crop productivity and jeopardize the food security of the growing world population. Predictions of climate change pose a continued increase in CO₂ in the atmosphere associated with higher temperatures, an increase in the duration and intensity of drought and more irregular rainfall patterns. This implies that the productivity of crops will be influenced by complex environmental interactions (increased atmospheric CO₂, increased temperature and drought), and the end result will depend on climatic factors soil conditions of the regions and the characteristics of the crops and even cultivars.

Therefore, climate change raises important scientific challenges for plant physiologists. Firstly, in order to predict the impact of climate change on crops and natural ecosystems, we need to expand and broaden our knowledge about the responses of plants to the environment. This knowledge will provide tools to minimize its potential negative impact.

Plants through photosynthetic activity function as excellent sinks of environmental CO₂ reducing the effects of climate change and contributing to the Kyoto compliance. Additionally, the produced biomass could have an energetic use. However, those perspectives can be altered by factors such as limitation of nutrients and water, temperature rise, salt stress and/or other factors related to the rise of CO₂ that can affect physiology and productivity of the plants.

Thus, the objective of this research group is focused on the analysis of different factors associated with climate change that affect physiology, growth and productivity of the plants in the nowadays changing environment such as atmospheric CO₂, water availability, soil salinization, NO₃⁻ availability, temperature, as well as interactions within them, plant-plant interactions and bacterium-plant associations. This broad objective will permit us to investigate 1) if the plants will be able to adapt to these new environmental conditions, 2) if as the result of these climatic changes it would be necessary to find new varieties of the species currently used in agriculture or whether it would even be necessary to find other species better adapted to the new climatic conditions.

Genomic resources

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www.genomic-resources.eus

KEYWORDS: Conservation and promotion of natural diversity, population genomics, association study, selective sweep, metagenomics, bioinformatics,.

"Genomic resources" is a Consolidated Research Group designated by the Department of Education, Universities and Research of the Basque Government (2010-2015). The group has 4 main research lines, where the analysis of the genome variations is applied to (1) improve the management of farms, semi-wild species and hunting land species, (2) improve the management of the marine environment, especially of fisheries and mariculture species, (3) identify genes associated with adaptive traits and traits of economical interest, (4) personalized medicine, and (5) understand the role of microbial communities in the environment.

To carry out our objectives we have specialized in the analysis of genetic markers (sequences, microsatellites, CNVs and SNPs), using the most advanced genotyping and sequencing platforms, including NGS technologies.

1. POPULATION GENOMICS

The aim of our research is to provide useful information in order to balance the use of animal resources by a growing human population while sustaining natural diversity.

We analyse the genomic variation on a number of species from three socioeconomically relevant sectors: (1) Apiculture: local populations of honey bee. (2) Domestic species: Latxa and Sasi-ardi sheep breeds, and (3) Fisheries: European anchovy, Albacore, European sardine, Atlantic mackerel, and tench. Our studies aim to elucidate the genetic structure of populations within species, to estimate the intra- and inter-population diversity, to assess hybridization and introgression, and to achieve a better understanding of adaptive processes on local populations. Additionally, under a food sector perspective, we develop traceability tools based on genetic markers in order to assign an individual to its population of origin.

We strongly believe that the implementation in conservation/promotion policies of the knowledge raised by our research will be greatly beneficial to protect natural diversity.

2. GENE IDENTIFICATION

The general objective of this research area is to better understand the relationship between the genotype and the phenotype by the identification of gene/networks involved in the phenotypic variability of human and animal traits.

We focus on economically important animal traits, such as resistance to bovine paratuberculosis, milk production in sheep, or growth trait in mariculture species. We also are interested on the genetic component associated to local adaptation in sheep, anchovies, and honey bees.

Besides of this, we also work on the identification of susceptibility genes to human autoimmune diseases (e.g. Antiphospholipid Syndrome, Rheumatoid Arthritis, and Systemic Lupus Eritemathosus) in order to generate genetic tools useful for diagnostic/prognostic in individualized human medicine.

3. METAGENOMICS

The general objective of this research area is to study the microbial community structure and functions over space and time to contribute to the sustainable conservation and management of socioeconomically important ecosystems and regional resources. Currently, we are working on three main research lines studying the microbial community associated with: (1) marine/estuarine habitats, (2) the socioeconomically important Txakoli wine, and

(3) honey bee.

We aim to develop an accurate, straightforward and cost-effective method for estuarine and marine plankton monitoring that could serve as an early detection of ecosystems climate changes and/or pollution. This information will help policy makers in promptly designing mitigation actions.

We also work on elucidating the role of honey bee gut and hive microbiome in honey bee disease and parasite susceptibility. The efforts made in this field will make a step-change in the current understanding of honey bee resistance or tolerance to complex diseases.

Finally, we study the microbial consortia that coexist in the grapevine producing Txakoli wine. Our aim is to infer the relationship of the microorganisms with plant growth, health, and organoleptic properties of wine. A more comprehensive view of the plant-microbe system is key for the sought manipulation of the plant microbiome to reduce the incidence of plant diseases, increase agricultural production and reduce chemical inputs resulting in more sustainable agricultural practices.

4. BIOINFORMATICS

The specialization of the Genomic Resources group on the analysis of the genome/transcriptome variation has led us to use next generation sequencing (NGS) platforms, whose speed and throughput have unprecedented increase last few years. The later has imposed high demands on the bioinformatics tools necessary to assess and analyse the large volumes of sequencing data generated. Therefore, the aim at the bioinformatics research line of the group is the development of new bioinformatics tools driven by the needs arising from our internal investigation in “omics”.

In addition, the Genomic Resources group offers at the UPV/EHU an international postgraduate course (own Master) entitled “Bioinformatics & “Omics”, jointly with the University of Bordeaux (www.genomic-resources.eus/bioinformatics). The Master degree is aimed for students and professionals with Bioscience background (Biology, Biochemistry, Biotechnology, ...) who want to learn clear bioinformatics procedures and data interpretation processes, and why not say, accelerate their research findings.

Ecophysiology of Plant Stress and Soil Contamination (EKOFISKO)

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INVESTIGADORES: Unai Artetxe, Raquel Esteban, Beatriz Fernández, Maite Gómez, Fátima Míguez,
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KEY WORDS: Environmental Stress, Biomarkers, Nutraceutic, Photoprotection, Phytoremediation, Soil contamination, Desiccation, Revegetation

Since 1990 The EKOFISKO group has developed research and teaching activities on physiological and ecophysiological aspects of natural and anthropic agents causing stress in plants. Our group is a consolidated research group of the Basque Government composed of 8 PhD and 2 PhD students.

This group has developed a variety of novel methodological tools: (i) determination of plant stress biomarkers, in particular those related to photoprotection and oxidative stress, (ii) set up of plant toxicity bioassays to determine the ecotoxicological effects of pollutants in contaminated soils, and (iii) implementation of physiological parameters to evaluate phytotoxicity or damage caused by natural stress conditions as extreme temperatures, drought, light intensity, nutritional disorders, etc. In collaboration with other groups, we have incorporated genomic methodologies with emphasis in differential gene expression and in the application of DNA microarrays to assess and monitor soil health in a multidisciplinary approach. Lastly, in cooperation with the Dept. of Physical Chemistry we have developed a procedure to study molecular mobility of photosynthetic tissues, which is relevant to understand the mechanisms that underpin tolerance to desiccation.

All these methodologies have been implemented in several more applied research areas:

- Determination of the role of photoprotective compounds and tolerance to stress conditions (natural or anthropic) with particular emphasis on the acclimation to extreme environmental conditions, such as those prevailing at high altitudes, forest understory or historically polluted sites.
- Use of plant biomarkers to monitor environmental and global change and genotype plant selection for tolerance to adverse climatic agents and phytoremediation.
- Identification of environmental agents to enhance nutraceutical compounds (carotenoids and tocopherols) in plant foods.
- Use of plants for ecological restoration of degraded environments, specially polluted soils through ecotechnologies as bio- and phytoremediation (phytostabilization, phytoextraction and rhizodegradation).
- Assessment and monitoring soil health with biological indicators during remediation processes.

The research indicated above is currently carried out in a multidisciplinary approach in collaboration with relevant national and international scientists, universities (Complutense de Madrid, Autónoma de Barcelona, La Laguna, Helsinki, La Frontera, Tartu, Australian National, Innsbruck, St. Thomas, etc) and institutions (Neiker, Gaiker, Phytosphere Institute, Royal Kew Gardens, USDA, etc), and supported regularly by many competitive projects. The quality of group's achievements is supported by regular publications in international journals (48 in the last 5 years), and by regular participation in national and international congresses. We also have a compromise on the cooperation for development, with several projects in Latin American universities (Chile, Nicaragua and Cuba). Besides, not only our group is very active in the formation of PhD students, but also we participate in three Official Master Programs: "Agrobiología Ambiental", "Environmental Contamination and Toxicology" and "Enología Innovadora" and in the Doctorate Program "Agrobiología Ambiental". The latter has been honored with a quality award by the Ministry of Economy and Competitiveness.

Group for the study of Microalgae at the University of the Basque Country

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Microalgae, Toxic Phytoplankton

Phytoplankton are the autotrophic component of the plankton community and the main responsible of primary productivity in the ocean. Furthermore, phytoplankton can be a source of problems, when toxic species are present or the density of the community is very high. This is the reason for monitoring the phytoplankton community along the Basque coast or in the Bilbao estuary. Due to the difficulty of identifying the organisms of the community with the monitoring routine techniques to a species level, in our laboratory some phytoplankton groups have been analyzed using some other different techniques. About Haptophytes and Cryptophytes, more than 20 species of each group have been isolated, describing the new species *Prymnesium palpebrale*, *Urgorri complanatus*, *Teleaulax minuta* and *T. gracilis*. Among diatoms, we have focused on the toxic genus *Pseudonitzschia*, identifying more than ten species, with *P. plurisecta* and *P. abrensis* as new species. Apart from the water column, microalgae can be found in the benthic zone, where toxic dinoflagellates have been studied during the last years with special attention due to the problems they can cause in tropical waters. At the Basque coast, we have detected the presence of genus *Ostreopsis*, which causes some toxicological problems at the Mediterranean Sea.

Cannabinoid (WIN 55,212-2) and chloral hydrate influence in *Calliphora vicina* (Robineau-Desvoidy, 1830) (Diptera, Calliphoridae) development and its implication in post-mortem interval estimation

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KEY WORDS: *Calliphora vicina*, Calliphoridae, cannabinoide (WIN 55,212-2), chloral hydrate, forensic entomology, entomotoxicology, larval development, temperature, post-mortem interval (PMI).

Entomotoxicology studies the influence of toxics in insect scavengers, identifies drugs and toxins present in contaminated tissues, in special when no cadaveric tissues are collected under suitable conditions to be analyzed. Entomotoxicology also studies possible effects caused by the presence of these substances on the development of arthropods, since they can also alter them, affecting the estimation of the postmortem interval (PMI). Insects, as living beings can be affected by toxins stored in their tissues and modify their development pattern, introducing miscalculations if the presence of toxins in their tissues is obviated. The increase in deaths related to drugs (mainly heroin and cocaine), accidents, murders or suicides due to poisoning and/or toxic substances justifies the great interest aroused to this discipline in forensic medicine. Many drugs can be detected analyzing insect tissues when collected as evidence. Thus, drugs such as heroin, codeine, methadone, cocaine, methamphetamine, ketamine, alcohol, barbiturates among others, have already been isolated from insect tissues. Therefore, the main interest of forensic entomotoxicology is to detect the use of drugs of abuse just before death, both to correctly estimate the PMI as well as to determine if the decease had previously consumed drugs.

For this study, we choose the blue bottle fly *Calliphora vicina* (Robineau-Desvoidy, 1830) as we have enough data about its development under laboratory conditions. We have also confirmed that it is the most frequent species of forensic interest in the Autonomous Community of the Basque Country (CAPV). This study is of great importance as it is one of the first species associated to the colonization of cadavers by necrophagous insects, being very useful to estimate the PMI based on the period of minimum activity of the insects (PIA_{min}). As many parameters affect insects development, accelerating, delaying and even stopping adult emergence. The development of this species under controlled conditions has been previously studied in the Forensic Entomology lab at the University of the Basque Country (UPV/EHU). Therefore, we focus this research on the effect of drugs in the development of *C. vicina*. That for, maggots were fed by carcasses of rats previously contaminated with WIN 55,212-2, a CB1 and CB2 agonist of cannabinoid receptors, and with chloral hydrate; populations were compared with maggots reared on rats only contaminated with chloral hydrate and with a control (non contaminated euthanised rat). These substances were administered to the rats intraperitoneally before slaughter. Diptera populations were reared at an average temperature of 21°C until adult emergence. Three parameters have been taken into account: development time, larval size and adult size. It has been observed that larvae developed in rats treated with cannabis and chloral hydrate suffer a one-day delay in pupation and adults emergence; specimens developed in rats just treated with chloral hydrate delayed only one day the emergence of adults in contrast to the development of the control population (no treatment). As far as larval size is concerned, a decrease in size was observed during the first four days of larval development in the two treatments respect to the control. However, there was an increase in size of larvae from day 5 onward, where the size of the specimens developed in rats with treatment was greater compared to the control specimens. Regarding the size of the adults, no major differences were observed. Male specimens developed on drugged rats are slightly longer than control males, but no significant difference was observed in females. To conclude, this study confirms the influence of cannabis on the development of blow fly larvae, which affects their development time and alters the estimation of the postmortem interval (PMI) introducing errors if previous consumption by the victim is obviated. Therefore, drug consumption and its effects should not be overlooked in future investigations on forensic entomology cases.

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Risk of graphene nanomaterials for the marine environment and human health

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KEY WORDS: Graphene oxide and reduced graphene oxide, cytotoxicity and sublethal effects, mussel hemocytes, and human pulmonary cells.

Graphene-based nanomaterials have been extensively explored as some of the most promising materials in electronics, energy and biomedicine due to their unique properties: two-dimensional planar structure, large surface area, chemical and mechanical stability, excellent conductivity and good biocompatibility. Graphene oxide (GO) nanoplatelets are one of the most important graphene derivatives and have been extensively studied in recent years. In order to improve GO electrical properties, nanoplatelets are chemically reduced to increase their conductivity. This reduced GO (rGO) shows different properties and behavior compared to GO and both have been increasingly used in many industrial products. In the last few years, the market for graphene-based nanomaterials is in exponential increase and it is expected that large quantities of graphene-based wastes will end up in the environment representing a risk for marine environment and human health.

In collaboration with the POLYMAT Institute and Imperial College London, the Consolidated Research Group “Cell Biology in Environmental Toxicology-CBET” at the Faculty of Science and Technology and Plentzia Marine Station (PIE) is using alternative toxicity testing methods to evaluate the risk of different nanomaterials, including GO and rGO, for the marine environment and human health. To assess the potential toxic effects of both GO and rGO nanoplatelets to marine organisms we used *in vitro* assays with mussel (*Mytilus galloprovincialis*) hemocytes, as these important immune cells have been successfully used to assess the toxicity of metal nanoparticles. To evaluate the risks of GO and rGO on human health, we used *in vitro* assays with highly relevant human alveolar type-I-like epithelial cells (TT1 cells). TT1 cells have been demonstrated to be sensitive to nanoparticle exposure.

In this study, we used a two-step procedure. The first step consisted in a screening of the cytotoxicity of GO and rGO (with and without polyvinylpyrrolidone (PVP) as stabilising agent) at a wide range of concentrations (0.001 to 100 mg/L) on both mussel and human cells. Toxicity of PVP alone was also tested and LC50 values were calculated for each case. In the second step, sublethal (<LC25 values) environmentally relevant concentrations were selected to perform functional tests in both cell types, evaluating the production of reactive oxygen species (ROS) and plasma membrane (PM) integrity. In addition, internalization of nanoplatelets was determined through TEM analysis in hemocytes and response of inflammatory mediators was assessed in TT1 cells. GO and rGO showed low and dose-dependent cytotoxicity to mussel hemocytes and human TT1 cells, rGO being slightly more toxic than GO. PVP was not toxic to any cell type but increased bioavailability of nanoplatelets. Both GO and rGO increased ROS production in mussel and human cells at sublethal concentrations. At the same time, GO and rGO caused a significant decrease in cell membrane integrity in both cells. In hemocytes, GO and rGO produced invaginations and perforations of the PM and were found in the cytosol and in endolysosomal vesicles. In TT1 cells, inflammatory mediator release was significantly increased after exposure to both GO and rGO nanoplatelets. In conclusion, GO and rGO are not highly cytotoxic for mussel and human cells but they trigger important cellular mechanisms leading to toxic responses. Chemical reduction of GO increased its bioreactivity possibly due to the restoration of its surface electronic structure. Finally, *in vitro* assays provide valuable and sensitive tools to detect differences in cellular reactivity of nanomaterials related to differential physico-chemical properties.

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Unveiling virulence mechanisms of fungal pathogens, the hidden human killers

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KEY WORDS: *Candida albicans*, *Lomentospora prolificans*, Immunocompromised, Cancer, Mannoproteins, Immunoglobulins

Our research group is interested in studying the virulence mechanisms of two fungi involved in systemic infections of immunocompromised patients. The first one, *Candida albicans*, is a commensal yeast that can form real hyphae and it is the most prevalent fungus in health-care associated infections. It is also related to inflammatory responses and tumour adhesion. The second one, *Lomentospora prolificans*, is an environmental filamentous fungus, mainly found in Australia and the Iberian Peninsula, which induces high mortality rates due to its inherent resistance to a wide variety of antifungals.

Regarding *Candida albicans*, our group has hypothesised that, in immunosuppressed patients, the inflammatory response produced by *C. albicans* in the hepatic endothelium may favour the adhesion of the tumour cells to the endothelial cells, leading to liver metastasis. We have identified the fraction of *C. albicans*, a mannoprotein fraction, that increases the tumour adhesion the most and lately, we have identified the mannoproteins within this fraction. We have proceeded to clone them in a bacterial model (*Escherichia coli*) and in an eukaryotic model (*Pichia pastoris*) in order to obtain them individually at high concentration. Afterwards, the proteins have been purified and they have been tested individually *in vitro* showing a prometastatic effect in a mouse hepatic endothelium. Two of the produced recombinant proteins, Kre9 and Adh1, have been selected and monoclonal antibodies against them have been produced. Currently, the ability of these antibodies to reduce the adhesion of tumour cells to mouse hepatic endothelium and their effect over the fungus is under study. Moreover, one of the obtained antibodies is able to recognize the hyphae, and not the yeasts, of *C. albicans* and it does not stain the hyphae of *C. dubliniensis*, the unique other fungus from *Candida* genus able to form true hyphae.

Lomentospora prolificans has been widely described as an inherently resistant fungus to all the antifungals used nowadays. Therefore, our research group have followed different study pathways in order to improve the treatment against the devastating infections caused by this fungus. In this sense, since the immune system status is critical for the establishment of *L. prolificans* infections, we have studied the humoral and innate responses of healthy and infected individuals. Thus, we are analyzing the humoral immune response during disease, both using samples from a murine model of infection and from patients suffering from these mycoses. Concerning the first, we have established a murine immunization and infection model that will help us to understand the role of humoral immunity during *L. prolificans* infections and to evaluate the possibility of a fungal vaccine as an alternative therapy for these mycoses. Furthermore, since this fungus shows a neurotropic behaviour when it gets disseminated through the bloodstream, we studied the role of microglia during these infections. To do that, we use both the BV-2 cell line and primary cell cultures, and we determined parameters such as phagocytic rate, cytokine and ROS production, etc., as well as the role of pattern recognition receptors (PRRs) of immune cells. Finally, given the fact that only the azole compound voriconazole, which is the first therapeutic strategy, presents slight effects on the fungus, we have studied the morphologic, ultrastructural and proteomic changes occurring in the fungus when exposed to voriconazole. Interestingly, we have identified some proteins that might be related to antifungal resistance. Therefore, we are producing knock-out strains of some of these targets in order to unveil their role in this process, and also in others such as fungal virulence.

Genomics, health and biotechnology

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KEY WORDS: genomics, obesity, gene-environment interactions, infectious diseases, animal models, vaccine adjuvants, autoimmunity

Our research interests include both human and animal health.

Human health: life style and genetics in obesity

Obesity and its associated comorbidities represent one of the biggest public health challenges today. The marked rise in obesity observed over the last years suggests that behavioral and environmental factors underpin the mismatch between energy intake and energy expenditure. Our main interest in human health is the disentangling of environment-genes interaction in relation to obesity in work environments.

During the 2011-2013 period, we have been involved in the OSAGEIN study (Osasuna+ Genetika+ Ingurumena).

The main objective of this study was to improve the health of people who work in our University. Furthermore, this study took into account the differential morbidity of women and gender segregation of work. To this end the gender perspective was incorporated in both the selection of variables to study and unbundled analysis of all the data. Beyond the biological characteristics associated with sex our research takes into account sociodemographic variables such as care of others, free time and overnight stay, that contextualize healthy or unhealthy environments.

Interesting aspects of this study were also:

- To provide data for the development of assessment tools that can be incorporated into occupational health surveillance.
- To suggest and provide guidance for interventions and programs to promote occupational health.
- The applicability of the study to other similar work environments

Animal Health: biotechnological applications and characterization of animal models of infectious diseases

In relation to animal health, we are involved in two main lines of research with biotechnological applications:

- ASIA syndrome. Ovine autoimmune/inflammatory syndrome induced by adjuvants, or ASIA syndrome, is a new entity linked to the repetitive inoculation of aluminium-containing adjuvant vaccines. The objective of this specific project is to reproduce the syndrome and perform a complete study of the effect of the alum adjuvant, including the most relevant aspects of the disease. Our group is in charge of the transcriptomic and miRNA analysis. This work could help to improve these vaccines.
- An animal model for human hepatitis. The Eastern woodchuck (*Marmota monax*), is a rodent species used as a surrogate animal model for research on HBV infection. Natural infection of woodchucks with woodchuck hepatitis virus (WHV) causes liver disease highly similar to that induced by HBV infection in humans thereby representing the closest pathobiological model for HBV. We are characterizing immune genes polymorphism in Eastern woodchuck as it could help to improve our understanding of HBV infection and disease development.

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Epidemiology of obesity

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KEY WORDS: obesity, environmental factors, genetic factors, image, birth weight, phenotype, case-control.

INTRODUCTION

Common obesity is an unfavourable condition characterized by a high body weight due to an excess of adipose tissue mass. It is caused by a positive balance between amounts of energy consumed over the energy spent.

Obesity is a complex multifactorial phenotype caused by genetic and environmental components and their interactions. Genetic factors are important in determining individual differences in body composition within a given environment, but they cannot explain the epidemic proportions of obesity and overweight reached in the last decades in many developed and developing countries. Environmental changes such as increased food availability and a more sedentary lifestyle may also explain the globally prevalence of obesity.

Obesity is one of the most complex and important public health problems and it is also a social illness indicator. It has been associated with the development of many metabolic alterations and health conditions such as impaired glucose tolerance, type II diabetes, hypertension and cardiovascular diseases, osteoarthritis, sleep apnoea, depression or even some kinds of cancer.

OBJETIVES

The main objectives of this research are:

1. Determine the relative influence of environmental factors, in different obesity phenotypes.
2. Analyse image and body composition according to different types of obesity and nutritional categories.
3. Identify susceptibility genes for obesity: association analysis of the different alleles of candidate genes with different phenotypes of obesity.
4. Analyse the association between birth weight and anthropometric measures related with body morphology and composition in childhood and adulthood.

METHODS

The collected data provided information about environment, phenotype and genetic profile of subjects. Two different samples were collected for two different study designs:

- **Case - Control (Sample 1).** Observational and retrospective study to determine the association between an event (obesity) and the exposure to risk factors (genetic or environmental). Subjects were selected based on their disease status as cases (obese) or controls (non-obese). Both groups were compared in relation to the studied factor by a binary logistic regression. Environmental factors were related to personal and family history, (in)activity, eating patterns, sleeping patterns, tobacco and alcohol. For genetic factors some SNPs from candidate genes were selected (e.g. TNF, FTO, MC4R, LEPR, UCP2).
- **Longitudinal cohort (Sample 2).** In this approach, a randomly selected sample in that subjects were not selected for any specific feature or trait, was used. The association between birth weight and anthropometric measures during growth were analysed by multiple regression analysis adjusted for different covariables (birth order, maternal age, etc.).

The programs used in this research were: SNPbrowser, SPSS v18.0, Microsoft Excel 2010, TaqMan Genotyper Software and Stata statistical software package v. 12.0.

URBAN ELIKA - elikagaiak denontzat

Transdisciplinary Research Group of Studies on Food and Society

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KEY WORDS: human right to food, food waste, social responsibility

Urban Erika - *Elikagaiak denontzat* (Food for all, in Basque language) is a Trans-disciplinary Research Group of the University of the Basque Country involved in Food and Society Studies. It aims to contribute to the remotion of the institutional, legal, socio-economic and technical obstacles that impede access to healthy and sufficient food in urban societies and is also committed to promoting a more responsible, sustainable and fair use of food resources. Some of its members have been working together since 2007, but URBAN ELIKA was formally created thanks to an agreement signed in 2014 with SORTARAZI - Claretian Association for Human Development (NGO). We face social challenges related with Food involving those work areas: (1) Governance and Food Law; (2) Logistics and Applied Mathematics; (3) Food safety and Immunology; (4) Human Nutrition and Food Anthropology; (6) Social Work, Social Psychology and Sociology.

We are encouraging master and degree final projects from an Innovative Educational Project 2014-2016, founded by the vice-rectorship for University Grades and Innovation of UPV/EHU via Educational Advice Service. The title of the project is “Cross Competences in dissertations of Food Inclusion. *Ethic and Social competences in Degree Final Projects of Social Responsibility against food poverty in the Basque Country: design, implementation and evaluation in a multidisciplinary team*”.

In 2015 more than one hundred experts from 16 countries (5 continents) took part in a Conference organized by Urban Erika. More than 70 authors contribute to the book “Envisioning a Future without Food Waste and Food Poverty: Societal Challenges”, Wageningen Academic Publisher.

Another initiative of *Urban Erika - Elikagaiak denontzat* is a Summer School named *Food Forum EHU*. Food Forum EHU is part of the Summer Courses of the University of the Basque Country. Critical analyses of current food systems underline the need to respond to important challenges in questions of nutritional health, environmental sustainability, socio-economic development and protection of the cultural wealth. This School has been designed as a forum where academics, stakeholders, social entities, students and citizens may reflect together on the decisions we individually and collectively make regarding food. We aim to raise awareness on the negative and promote transformation towards a more sustainable, healthy and fair use of food resources. Human right to food, sustainability, food sovereignty, local development or food health are some of the issues that arise at Food Forum. The Summer Course offered in 2016 faces the Challenge of Making Use of Unmarketable Food.

Current research lines:

- 1) Human right to food and Food Sovereignty.
- 2) Sustainable food production and consumption.
- 3) Transforming food waste into valuable products (circular economy).
- 4) Improving access to food in urban societies (food recovery, nutritional care, social inclusion).
- 5) Consumer concerns related to new food and controversial food (functional, transgenic, etc.).
- 6) Strategies that aim to promote responsible food consumption (nutritional, environmental and/ or social

Understanding disorders of the visual system and promoting repair and regeneration

Neuro-ophthalmo Biology Group

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KEY WORDS: retina, glaucoma, cornea, uveitis, tears, neuroprotection, retinal ganglion cells, glia, computational, ocular surface, primary cell cultures.

We are a multidisciplinary group consisting of ophthalmologists, biologists, biochemists, physicists and veterinarians and currently have 15 members. We have been working together for the last 22 years. Our group has been recognised by the Basque Government as a consolidated group. Our lab is located in the Faculty of Medicine in the Department of Cell Biology and Histology but members of the group also work in Hospitals such as Cruces, San Eloy, Donostia and Txagorritxu. The director of the group GOBE (Grupo de Oftalmo-Biología Experimental) www.ehu.es/GOBE is Prof. Elena Vecino from the Faculty of Science and Technology.

Within GOBE there are four main areas of research:

1. **Neuroprotection** of retinal ganglion cells by retinal glia (PI: Prof. Elena Vecino). Understanding the molecular mechanisms that lead to the death of retinal ganglion cells (RGCs) in retinopathies such as **glaucoma, the first cause of blindness over the world**. RGCs are neurons that transport visual signals from the retina to the brain and their loss, after disease or injury, leads to irreversible blindness. By studying the molecular interactions between RGCs and glia, which are the supportive cells of the retina, we hope to understand how we can prevent cell death and instead promote RGC regeneration. In this project we collaborate with researchers at the University of Salamanca, Cambridge University and New York Medical College as well as several biotech companies like IMG and Neuroprot in several projects. The **computational** non-invasive characterisation of cellular changes within the normal and pathological retina is an aspect that the group is interested in and we are currently collaborating with physicists.
2. **Ocular surface tears** (PI: Dra. Arantxa Acera). Focussed on researching factors present in the tears, that can promote the repair of the injured ocular surface, in particular the corneal epithelium. In this project we have been collaborating with several Depts. at the FCYT of the UPV/EHU: Organic Chemistry, Fisiology, Biochemistry, Physical Chemistry, as well as SGiker for the lipidomic project. Previous results and patents are at present used to develop a Tear Monitor that will be soon in the market.
3. **Analysis of aqueous humor in glaucoma patients** (PI: Dr Javier Haritz Urkola). Analysing the viscosity of aqueous humor in patients with glaucoma to detect any changes compared with healthy patients. Alterations in its composition by metabolomics and Biophysical properties has helped us understand more about how glaucoma progresses. We are collaborating in this project with OWL-genomics company and Copenhagen Hospital (Dr. Cabrerizo).
4. **Uveitis** (PI: Dr. Alex Fonollosa) Uveitis is a general term describing a group of inflammatory diseases that produces swelling and destroys eye tissues. Dr Alex Fonollosa's group are interested in understanding more about uveitis and are currently studying retinal cell cultures to test the possible action of somatostatin in the tight junctions formed in the retina-pigment epithelium. These basic studies are done in collaboration with SGiker and biotech companies with the aim of developing clinical applications.

Together we have a shared interest in studying disorders of the visual system using different approaches with the final idea to translate to the patients our discoveries, thus we are currently working with industry. In the last 6 years a total of 10 PhD theses and 30 peers review papers Q1 have been published by members of GOBE.

Integration of ecosystem services in a sustainable land management

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KEY WORDS: Ecosystem services, Indicators, Mapping, Models, Participatory process, Perception, Scenarios.

The aim of our research group is to analyze the structure and functioning of the socio-ecosystems in order to provide the information and tools required by the decision-makers for a sustainable land management. A sustainable management must value, maintain and improve ecosystems and their global change adaptability to promote society well-being.

In this context, we are performing the following actions:

1. Identification and analysis of state and evolution of ecosystem services in the last decades by means of 60 indicators.
2. Mapping ecosystem services at different spatial scales (CAPV, Bizkaia, Lea watershed, Urdaibai, Bilbao Metropolitan Greenbelt...), using GIS programs. Some of these services are: Carbon storage, Water Flow Regulation, Natural diversity conservation, Recreational use, Aesthetic quality of landscape...
3. Use of models to develop future scenarios to analyze the consequences of the decisions on the flow of ecosystem services.
4. Analysis of perception and demands by society of ecosystems services, by means of participatory processes.
5. Analysis of the applicability of the information generated in the project: mechanisms and pathways to integrate this information into the decision-making processes.
6. Development of new tools to facilitate decision making: multi-functionality indicators.
7. Disclosure of the concepts and results.

Acknowledgments

We are very grateful to the financial support from the Department of Environment of the Country Council of Biscay (Millennium Ecosystem Assessment of Biscay Project) and from the Department of Environment and Landscape Policy of the Basque Government (Millennium Ecosystem Assessment of Basque Country Project).

Sport Genomics Research Group

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KEY WORDS: Sport, Genetics, SNP, trainability, injury, polymorphism, performance, Nutrigenetics

SPORT GENOMICS IN A FEW WORDS

Sport Genomics is a research Group actually focused in studying genetic factors associated with personal injury risk, trainability and the response to nutrition.

According to a number of heritability studies, Genetics influences 30-80% of the Human variability to respond differently to each training program or to each kind of diet. Thus, determining genetic markers associated with this variability, would not only improve performance of elite athletes and would reduce their injury risk in a natural way, but also would have a great positive impact in public health, as it would promote general population to acquire and maintain genetically individualized healthy habits, by preventing unsuccessful strategies.

Therefore, our aim is to develop genetically personalized training and nutrition programs, by a whole genome screening of markers associated with the variability in response of training programs of three types of sports focused respectively on power, endurance, and power-endurance.

INTERACTIVE R&D: AN INNOVATIVE CONCEPT

Research activity of Sport Genomics is usually done in collaboration with K-DNA Genomics enterprise, a spin-off of the University of the Basque Country, which invests nearly the 100% of its profit to University R&D. K-DNA Genomics is focused on Development of Bio-technological solutions for Sport Sciences, in three interconnected areas: sport specific Genetic Analysis and Online Apps; R & D applied to the Genetics and Nutrition; and Education in Nutrition and Sport Genetics. Sport Genomics and K-DNA Genomics collaborate through an innovative concept called “Interactive R&D”.

In interactive R & D, the athlete becomes an active agent in R & D related to Development and continuous improvement of his own Genetic Analysis, donating his genetic results anonymously, performing physical tests and completing questionnaires through the exclusive online application.

In this way, in interactive R & D the participating athletes collaborate directly with researchers and sports professionals, invest in the improvement of the R&D, and in the permanent updating of the Genetics Services which they themselves enjoy.

VISION

Our vision can be summarized in promoting:

- Innovation and practical applications in Nutrition and Sport Genetics, improving the performance, health and quality of life of athletes and the general population.
- Science culture in society, opening a new channel of technology transfer, communication and cooperation between researchers, sports professionals and athletes.

Analysis of mechanisms involved in bacterial adaptation to stress and their regulation by antisense RNAs

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KEY WORDS: small RNAs, RNase E, post-transcriptional control, *Vibrio harveyi*, *Escherichia coli*, bacterial stress responses.

The ubiquitous presence of microorganisms is largely associated with their unique abilities to adapt and strive in adverse environments. We use the Gram-negative bacteria *Escherichia coli* (*E. coli*) and *Vibrio harveyi* (*V. harveyi*) as model organisms to study post-transcriptional mechanisms controlling mRNA stability as well as regulation of these mechanisms by environmental signals. Our three major lines of research are briefly outlined below.

1. High-throughput screening of antisense RNAs with new roles in *E. coli* stress responses

Recent studies revealed a new class of small antisense RNAs (sRNAs) that play important roles in regulatory mechanisms that enable *Escherichia coli* (*E. coli*) and other bacteria (including essential genera of pathogenic enterobacteria) to adapt to environmental stresses. Given important functions of sRNAs in bacterial adaptation and virulence, the main goal of this subproject is to employ a combination of high-throughput biochemical, genetic and molecular biology approaches and characterize a large fraction of experimentally identified and *in silico* predicted sRNAs that have not been studied previously.

2. Identification of regulatory factors playing the key role in the temperature-dependent adaptation of *Vibrio harveyi* in aquatic systems

Here we study the effect of environmental factors (starvation, temperature, exposure to predators and solar radiation) on the long-term adaptation of several *Vibrio* species (namely, *V. harveyi*, *V. tubiashii*, *V. cyclitrophicus* and *V. kanaloae*) recently isolated from the coastal water of the Biscay Bay. The aim of this study is to find a link between the adaptation phases (associated with distinct phenotypical and physiological changes) and the corresponding regulatory mechanisms controlling gene expression in *Vibrio* species.

3. Subcellular localization and protein-protein interactions of glycolytic enzymes in *E. coli*

Our previous work has shown that the glycolytic enzyme enolase is a major component of the degradosome, a multienzyme complex controlling RNA processing and decay in *Escherichia coli* (*E. coli*) and additionally containing RNase E (Rne), the exoribonuclease PNPase (Pnp) and DEAD-box helicase RhlB (RhlB). While association of RNase E with RhlB and PNPase was shown to be critical for the normal efficiency of the degradosome-mediated RNA decay, the function(s) of enolase in the degradosome remains uncertain. The long-term goal of our study is to perform in-depth analysis of the protein-protein network that control glycolysis and link this process to RNA turnover and sugar transport in *E. coli*.

Some of the most recent results include:

- Identification of stress-related genes and their products (e.g. genes encoding transporters, transcription factors and essential metabolic enzymes) important for adaptation of *V. harveyi* in natural aquatic systems;
- Observation that *Vibrio harveyi* persistence in seawater microcosms involves up- and downregulation of several known and putative small RNAs;
- Development and testing of custom microarrays for efficient gene expression profiling of *E. coli* sRNAs and their mRNA targets.

Human Molecular Evolution

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KEY WORDS: Neanderthal, archaic and modern humans, Next Generation Sequencing, Paleogenomics, bioinformatics, skin pigmentation, melanoma, genetic expression, human diversity, resequencing, aptamer

PALEOGENOMICS: RECONSTRUCTION OF THE HUMAN EVOLUTIONARY HISTORY

The aim of the paleogenomic research is to understand the evolutionary process of our species. The development of the Next Generation Sequencing (NGS) techniques allows the comparison of the genomic data of our species with other closely related extinct species as Neanderthals and other archaic humans. Paleogenomics analysis contributes to understand the evolutionary success of our species from Middle and Upper Palaeolithic as well as to analyze the influence of environmental and cultural factors on genomic human evolution. For this purpose, we are identifying the specific genomic variants of the first *Homo sapiens* in Europe (35.000 years ago) comparing this and another paleogenomes with contemporary human species genomes to obtain direct evidence of migratory phenomena taken place during Upper Paleolithic. On the other hand, paleogenomics contributes to the knowledge of the genomic variation existing in the past both intraspecific and interspecific level.

PIGMENTATION OF SKIN AND MELANOMA

There are genetic and environmental factors that determine the risk to melanoma susceptibility. In particular, light-skinned individuals are less protected against photocarcinogenesis and/or photoaging after solar irradiation, especially in recent years, when UV radiation has increased due to the weakening of the ozone layer. Therefore, we are trying to identify genetic variation associated with skin pigmentation in humans, in order to infer its adaptive value and assess its biomedical implications. For that reason, we are focusing on the detection of differentially expressed genes in melanocytic cell lines from individuals with different skin pigmentation, using expression chips (Affymetrix). Subsequently, a subset of loci is selected to analyze their sequence diversity by resequencing and their variation in the copy number of their exons. The variability discovered is analyzed in collaboration with other laboratories, in melanoma patients and healthy individuals. We are evaluating the adaptive value of these polymorphisms by means of bioand trying to infer the potential biomedical implications (predisposition to cutaneous melanoma). On the other hand, we design aptamers, single-stranded oligonucleotides that bind with high affinity to the *α-MSH* hormone, a ligand of *MC1R*. These aptamers will allow the detection and the quantification of the hormone in individuals of light and dark skin pigmentation, and they may also serve as tumor markers for clinical diagnosis of melanoma.

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Ceramide kinase is implicated in spontaneous pancreatic cancer cell migration.

Enhancement of cell migration by exogenous C1P

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KEY WORDS: Chemotaxis, metastasis, sphingolipids.

Pancreatic cancer is the fourth leading cause of cancer mortality with a 5-year survival rate of only 6%. This aggressive disease is characterized by invasiveness, rapid progression and profound resistance to treatment. We showed recently that ceramide 1-phosphate (C1P) potently induced macrophage migration and that this effect was completely abolished in the presence of pertussis toxin (PTX), suggesting the participation of a G_i protein-coupled receptor in this process. Using an *in vitro* cell migration assay we show in the present work that human pancreatic cancer cells can migrate spontaneously and that exogenous C1P enhances spontaneous cell migration. Interestingly, spontaneous cell migration was insensitive to treatment with PTX. Investigation into the mechanisms responsible for spontaneous migration of the pancreatic cancer cells revealed that ceramide kinase (CerK) was a key enzyme in the regulation of this process. In fact, inhibition of CerK activity with the selective inhibitor NVP-231, or by treatment with specific CerK siRNA to silence the gene encoding this kinase, potently reduced migration of the pancreatic cancer cells. By contrast, overexpression of CerK stimulated cell migration, an action that was concomitant with prolonged phosphorylation of ERK1-2 and Akt, which are kinases involved in C1P-stimulated cell migration/invasion processes. We also show that these kinases are implicated in the enhancement of cancer cell migration by exogenous C1P. It can be concluded that CerK/C1P plays a critical role in spontaneous pancreatic cancer cell migration, and that targeting CerK expression or activity may be a relevant factor for controlling pancreatic cancer cell dissemination.

Funding: This work was supported by grant IT-705-13 from “Departamento de Educación, Universidades e Investigación”, Gobierno Vasco (Basque Government, Vitoria-Gasteiz, Spain).

Identifying the substrates of Ube3a the enzyme involved in Angelman syndrome

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Angelman Syndrome (AS; #105830), is a rare neurodevelopmental disorder that affects about 1/20000 births. It is characterized by: severe developmental delay, speech impairment, movement or balance disorder and behavioral uniqueness: frequent smiling.

Angelman Syndrome is mostly caused by a maternal deletion of the 15q11-q13 chromosomal region. Various genetic mechanisms can lead to AS, but mutations affecting the gene *UBE3A*, and more specifically just the activity of its product, the ubiquitin E3 ligase UBE3A enzyme, are sufficient to cause the syndrome. Here we present a strategy used to identify some relevant substrates of the UBE3A enzyme, using the fly *Drosophila melanogaster*.

Ube3a directly regulates several proteasomal interacting proteins through ubiquitination. Among the proteasome-associated proteins, only Rpn10 is degraded upon Ube3a overexpression. Ube3a dependent Rpn10 degradation affects the ubiquitination and degradation of other proteins. Our results place Ube3a as a Master regulator of protein homeostasis and provide new mechanistic insights for better understanding of the Angelman syndrome.

Transcriptomic studies to understand the *Aspergillus fumigatus* infections

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KEY WORDS: *Aspergillus fumigatus*, AWAFLUGE, infection models.

Aspergillus fumigatus is one of the most prevalent airborne pathogenic fungus. Despite immunocompetent hosts do not develop illnesses, in immunocompromised patients the inhalation of its conidia can result in allergic or invasive diseases. Among them, the most severe form is invasive aspergillosis (IA) with mortality rates of 70-90%, which are mainly due to the weakened immune system of the patients, the virulence of the fungus and late diagnosis. In addition, several studies have demonstrated that the pathogenesis of this fungus is multifactorial owing to a combination of its biological characteristics and the immune status of patients.

PURPOSE

- Improve the knowledge of the molecular factors involved in the virulence of *A. fumigatus* which might be useful to design new therapeutic strategies.

GENERAL TECHNIQUES

- Conventional microbiological techniques.
- Immunological and histological techniques.
- DNA and RNA extraction, reverse transcription quantitative PCR.
- Sequencing and bioinformatics.
- Animal model and cell line infections.

TRANSCRIPTOMIC TECHNIQUES

To carry out with the purposed above, the group developed an own whole genome custom microarray, known as AWAFLUGE v.1, in order to perform different transcriptome assays. Nowadays, two types of experimental infection models using the pathogenic mold *A. fumigatus* have been implemented in the laboratory routine:

- *In vitro* infections using a macrophage cell line and an alveolar epithelium cell line (for being the two cell types predominant in lungs) to study the fungal cell interaction.
- *In vivo* mice infection model developing an intravenous model and an intranasal model, in order to study the disseminated form of the infection, known as invasive aspergilosis.

GROUP PUBLICATIONS

- Abad *et al.* *Medical mycology* 51:545-554 (2013)
- Ramirez-García *et al.* *PLOS ONE* 8(1): e53584 (2013)
- Sueiro-Olivares *et al.* *Microbiology* 161:490-502 (2015)
- Pellón *et al.* *Journal of Proteome Research* 15: 595-607 (2016)
- Ramirez-Garcia *et al.* *Critical Review in Microbiology* 42: 181-193 (2016)

GROUP PATENTS

- Fernandez *et al.* N. de solicitud: P201131497 (15/11/2011) Entidad titular: UPV/EHU.

Acquired plasmids have a role in the fitness and phenotypic characteristics of bacteria

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KEY WORDS: antibiotic resistance, competitive fitness, conjugative plasmids, exogenous plasmid isolation.

The spread of antibiotic resistance among bacteria has become one of the most important health problems nowadays. The problem relies on the dissemination of antibiotic resistance genes by conjugative plasmids. Increasing antibiotic concentrations in clinical and natural environments enhances this problem. Many antibacterial compounds have their roots in natural environments, such as soil. As a consequence, bacteria have coevolved and shared resistance mechanisms and genes along evolution. This work is focused on the search of new conjugative plasmids from environmental unique soils in which high concentrations of antibiotics are present as a result of animal manure amendments. Additionally, we aim to study the effect of these plasmids on the fitness and phenotype of recipient bacteria.

Exogenous Plasmid Isolation technique was used to collect conjugative plasmids from the bacterial community present in different soils. We obtained a total of 17 *E. coli* transconjugants from 10 different soils selected with ampicillin, erythromycin, chloramphenicol or streptomycin. To study the effect that the acquisition of these plasmids has on the fitness and phenotype of *E. coli* transconjugants, we determined growth curves, antibiotic MIC values, and community-level physiological profiles (BIOLOGTM) which provide information on carbon substrate utilization patterns. We conclude that acquired conjugative plasmids affect both fitness and phenotype of recipient bacteria.

FISIKA ETA INGENIERITZA ELEKTRONIKA

FÍSICA E INGENIERÍA ELECTRÓNICA



Group of Magnetism and Magnetic Materials - BCMaterials

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KEY WORDS: magnetism, magnetic materials, nanoparticles, nanostructured materials, magnetoactive materials.

The Group of Magnetism and Magnetic Materials was established in 80's and is focused on the synthesis and characterization of magnetic materials with different technological applications. Nowadays, we are working on the following main research areas:

1. Nanostructured magnetic materials.
2. Magnetic Nanoparticles
3. Magnetoactive materials

One of the specific activities of the group and common to all the research lines is the use of large facilities around the world, such as neutron sources (ILL and ISIS) or synchrotron radiation (ALBA, Elettra, ESRF, Spring-8 and APS).

NANOSTRUCTURED MAGNETIC MATERIALS

This research area is focused on the preparation of magnetic nanostructures in thin films by sputtering. The main goal is to obtain nanostructures with magnetic and magnetotransport properties for its use in the design of sensors. The process to follow is the preparation of thin films and their subsequent magnetic and structural characterization, involving the study of their basic properties. Some studied materials are: a) Nanogranular transition metal (Mt) - noble metal (Mn) thin films (where Mt=Cr,Fe,Co,Ni; Mn=Ag,Au) with Giant-Magnetoresistent properties; b) Rare earths/Transition metals multilayers with typical Spin Valve features; c) Sandwich structure multilayers $[\text{Fe}_{20}\text{Ni}_{80}/\text{Ti}]_n/\text{Conductor}/[\text{Fe}_{20}\text{Ni}_{80}/\text{Ti}]_n$ for Giant Magnetoimpedance studies; d) nanostructured films fabricated by *nanosphere lithography* and *nanoporous alumina template lithography* techniques.

MAGNETIC NANOPARTICLES

Magnetic nanoparticles have been subject of intensive research due to their interesting properties suitable in numerous applications of very diverse areas: environment, electromagnetic radiation protection, biomedicine or data storage among many other areas. One of the main challenge to be faced is to be able to obtain high amounts of nanoparticles with the right composition, size and shape, narrow size distributions and surface which can be easily functionalized for their future applications. This group addresses the task in two different ways: a) the synthesis of nanoparticles by culturing magnetotactic bacteria "*Magnetospirillum gryphiswaldense*", obtaining nanoparticles with highly biologically controlled properties, and b) by electric explosion of wire, which leads to high amounts of magnetic nanoparticles.

Moreover, due to their potential use in magnetic memory and biomedical applications, in the last years the group has been also interested in the synthesis and characterization of permalloy nanodisks in magnetic vortex states prepared by colloidal lithography.

MAGNETOACTIVE MATERIALS

Magnetoactive materials are those that actuate in the presence of an applied magnetic field. In this area, we specially pay attention to two sort of magnetoactive materials: shape memory alloys and magnetostrictive materials, and magnetoelectric hybrid composites derived from them.

Software Technologies Working Group (GTTS, <http://gtts.ehu.es>)

Germán Bordel, Mireia Diez, Mikel Peñagarikano, Luis Javier Rodriguez and Amparo Varona
Department of Electricity and Electronics.

KEY WORDS: Information Retrieval for Multimedia Resources, Language and Speaker Recognition/Verification, Automatic Speech Transcription, Automatic Video Subtitling/Captioning

Research at GTTS focuses on fundamental software technologies, in particular those related to speech processing and information retrieval. We are working on speech segmentation, language and speaker recognition/verification, speaker diarization, automatic speech transcription, video subtitling, etc. Part of our efforts are devoted to develop tools and prototypes for various applications:

1. The spoken document retrieval system (Hearch: <http://gtts.ehu.es/Hearch/>) which looks like a conventional search tool (such as Google, Bing, etc) but is designed to retrieve audio/video segments based on the automatic transcription of speech contents (broadcast news repositories in Spanish and Basque).
2. The automatic bilingual video subtitling applied on the plenary sessions videos that the Basque Parliament posts in its website (<http://www.parlamentovasco.euskolegebiltzarra.org/>), running from September 2010.

Finally, we also devote great efforts to academic training (doctoral thesis and master), dissemination of results (both in prestigious publications and through technology transfer to companies in our area) and collaboration with other research groups.

RESEARCH ACTIVITY IN THE LAST FIVE YEARS

- UPV/EHU Research Group: 2013-2016 (37.000 euros)
- Projects, contracts and research fellowship: 10 (320.000 euros)
- Publications: 36 (8 JCR journals, 28 peer-reviewed conferences)
- Thesis: 3 presented
- Organization of international Workshops:
 1. Odyssey 2016: The Speaker and Language Recognition Workshop (<http://www.odyssey2016.org>)
- Organization of international competitions:
 1. Albayzin 2012 Language Recognition Evaluation
 2. MediaEval⁽¹⁾ - The Spoken Web Search Task (SWS) in 2013
 3. MediaEval⁽¹⁾ - The Query-by-Example Search on Speech Task (QUESST) in 2014.
 4. MediaEval⁽¹⁾ - The Query-by-Example Search on Speech Task (QUESST) in 2015.
- Participation in international competitions:
 1. NIST⁽²⁾ Language Recognition Evaluation (2011)
 2. NIST⁽²⁾ Speaker Recognition Evaluation (2012)
 3. NIST⁽²⁾ Open Keyword Search Evaluation (2013)
 4. NIST⁽²⁾ Language Recognition Evaluation (2015)

TECHNOLOGY TRANSFER

- Hitzaldi: tool for audio-text alignment in parliamentary interventions.
- Sautrela: software package (free access) for the development of speech processing applications.
- Hearch: search tool for audiovisual resources (from automatic transcriptions of speech)
- Kalaka-3: database for the development of language recognition systems.
- ICT- COST 278: database of TV news in Spanish and Basque for audio segmentation and speaker diarization.

⁽¹⁾ MediaEval Benchmarking Initiative for Multimedial Evaluation.

⁽²⁾ NIST: National Institute of Standards and Technology.

Automatic Control Group GAUDEE

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Departamento de Electricidad y Electrónica, Facultad de Ciencia y Tecnología, UPV/EHU;

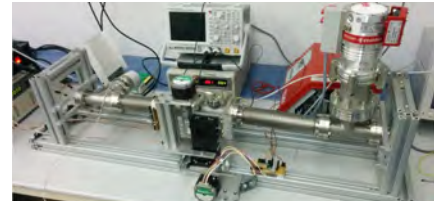
KEY WORDS: RF control, beam diagnostics, particle accelerators, EPICS, smart materials

The automatic control group of the University of the Basque Country (UPV/EHU), GAUDEE, is composed of academics and researchers whose labour is centered in the research and development of new advanced automatic control systems and techniques, combining the theoretical work with practical interest applications. The research activities of the GAUDEE group are very broad but two main research lines can be currently highlighted. The first one refers to solutions in the field of Particle Accelerators, both for basic and applied science and technology. This is carried out in collaboration with the RF and Microwave group of the Department of Electricity and Electronics in the joint IZPILab Beam Laboratory. The activities here include the development of beam diagnostics, RF devices and controls, and the corresponding electronics. A second research field is devoted to developing new advanced sensors and actuators, such as smart material-based actuators and sensors based in RF resonant cavities.

PARTICLE ACCELERATOR SCIENCE AND TECHNOLOGY

The group is involved in several projects for particle accelerators. Among these it is worth mentioning:

- Beam diagnostics and related electronics: active projects are related with Beam Position Monitors (BPM), for high-accuracy measurement of the position of beam particle bunches, key issue for subsequent stages of acceleration. The development of a digital data acquisition system for the BPM is truly challenging due to the high signal frequencies typically used in particle accelerators. This has been solved using fast DAQ devices, based on FPGA technology in conjunction with non conventional sampling techniques such as undersampling.
- RF systems: The RF system is an essential part of any particle accelerator. Its main task is giving energy to the beam. Besides, the RF system has a key role in the stability of the particle beam. A typical RF plant in an accelerator consist of an RF amplifier, a waveguide system, an RF cavity and a Low-Level RF (LLRF) control system. The LLRF developed by the group consists of an amplitude loop and a phase loop to regulate the amplitude and phase of the cavity accelerating voltage, and a tuning loop that regulates the resonant frequency of the cavity. The LLRF is developed purely digital and is based on IQ modulation and demodulation techniques. The amplitude of the cavity accelerating voltage is regulated with a precision of $<1\%$ and its phase accuracy obtained is $<1^\circ$. In this field we have started a collaboration with the FETS project of Rutherford Appleton Laboratory (Oxfordshire, UK) to integrate a new digital LLRF.



SMART MATERIAL BASED ACTUATORS

Ferromagnetic shape-memory alloys (FSMAs) are special smart materials that can undergo huge deformations, have a very fast response and can work at high frequencies when activated through a magnetic field (with the advantage of contactless activation). The group has built, controlled and tested several new prototype actuators based on FSMA monocrystals grown in-house. The latest activities on this line are aimed at saving operation energy by exploiting the "set and forget" properties of FSMA through event-based control techniques.

RF RESONANT CAVITY BASED SENSORS

Resonant cavities are closed conductive surfaces where the electromagnetic waves are constantly reflecting. Changes in their geometry result in electromagnetic variations, more specifically in the resonance frequency the cavities. The group is active in developing new sensors based on these principles. In particular the group has patented a new displacement sensor composed of two copper resonant cavities whose dimensions change in opposite directions by means of the displacement of a piston. Slight changes in position result in huge resonance frequency shifts that are easily measurable. This way, the results show that this kind of device can be used as a highly linear and sensitive nanometric precision displacement sensor. Other kind of sensors based on these principles are currently under development.

Structural Stability of the Hybrid Organic-Inorganic Perovskite Like - Cobalt and Cadmium Formate Crystals

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Metal Organic Framework, Phase Transition, domains

Crystals of Co-formate - $\text{Co}(\text{HCOO})_3[(\text{CH}_3)_2\text{NH}_2]$ and Cd-formate - $\text{Cd}(\text{HCOO})_3[(\text{CH}_3)_2\text{NH}_2]$, belong to a family of hybrid materials with metal - organic framework (so-called MOF-s). The members of this family have been intensively investigated in last years given their interesting physical properties (structural versatility, flexibility of metal-organic frameworks, phase transitions, multiferroic, magnetic, catalytic and gas storage properties) and in consequence their potential applications [1,2].

The crystals, used in this study, were grown from the mother water by slow evaporation at steady-state condition at 300K. Mother waters for Co-formate crystal growth were prepared under solvothermal conditions, using a mixture of $\text{CoCl}_2 \cdot 4\text{H}_2\text{O}$, DMF and H_2O . In the case of the Cd-formate the mother water was a mixture of two solution (HCOOH and $\text{NH}(\text{CH}_3)_2$ in CH_3OH and CdCl_2 in CH_3OH). The obtained crystals displayed a prismatic shape with a long edge of about 2 mm. They are thermally stable up to 395K and 385K for Co-formate and Cd-formate respectively. DSC measurements and ferroelastic domains observations show the existence of a phase transition in Co-formate crystals. Single crystal X-Ray measurements confirm this phase transition from a rhombohedral structure (R-3c) to a monoclinic ferroic phase (Cc) [3]. No structural change was observed in Cd-formate crystal in the temperature range 20K to 320K. The phase transition in Co-formate crystal can be described as an ordering process in which DMA cations fix their position within the cavities of the metal-organic framework. This freezing is also supported by dielectric and modulated temperature DSC measurements. The main differences in the structural stability of both compounds can be explained through a symmetry mode analysis of the distortion that provokes the deformation of the metal-organic framework and fix orientation of the guest molecules.

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Theoretical and Phenomenological Cosmology

J.M. Aguirregabiria¹, D. Brizuela¹, T. Broadhurst^{1,2}, N. Cipriani¹, I. de Martino¹, A. Feinstein¹, I. Garay¹, A. Garcia-Parrado Gomez-Lobo¹, J. Ibáñez¹, P. Jimeno-Romero¹, R. Lazkoz¹, I. Leanizbarrutia¹, M. Ortiz¹, J.M.M. Senovilla¹, B. Reina¹, R. Vera¹, J. Viegas¹

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Cosmology, General Relativity, modified theories of gravity, dark matter, dark energy, gravitational lensing

This line of work focuses on several theoretical and phenomenological aspects of the Universe, both in the context of General Relativity and in the wider context of modified theories. This is an area of research in full swing thanks to the arrival of new observational data. Broadly speaking these data provide surprising conclusions about the possible components of the Universe, whose "presence" is manifested in the kinematics of the Cosmos at different scales. One of the most controversial features is the apparent acceleration of the expansion of the Universe.

Two main sublines:

- Dark matter and energy: observational tests and alternative gravity theories
- Gravitational lensing, galaxy formation and galactic clusters, panoramic surveys and galactic telescopes.

Physical and mathematical fundamentals of the structure of the Universe

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Cosmology, General Relativity, Loop Quantum Gravity, Relativistic Astrophysics, neutron stars, black holes, gravitational waves

Einstein's equations of General Relativity (or modifications) link the geometry of spacetime (gravity) with the physics of non-gravitational fields. They constitute the framework for the study of the Universe and relativistic astrophysical objects. A better understanding of the Universe involves deepening the description of its early stages, regimes of high energies, and the principles governing the laws that govern it. Cosmology and physics directed to the description, evolution and emission of gravitational waves of relativistic systems are intimately related to the rest of the aspects of the structure of the Universe, that is to say, with more fundamental aspects, and in general of a more mathematical nature.

Main sublines:

- Dynamics of very compact astrophysical objects and black holes. Emission of gravitational waves, and cosmological gravitational waves. The role of the cosmological constant.
- Quantum cosmology and loop quantum gravity: dynamics, semiclassical approach and physical consequences.
- Mathematical relativity; trapped and umbilical submanifolds, computer algebra, initial data characterisations and exact solutions.

QUINST - Quantum Information, Science and Technology Group

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KEY WORDS: quantum devices, quantum information, quantum metrology, quantum simulations

Quantum theory is at the heart of modern technology. Our group explores several domains of quantumness at the frontier of current knowledge, actively seeking opportunities to design new devices or operations in areas such as quantum simulation, metrology, or information processing. Our research ranges from fundamental studies to more applied and directed investigation for efficiently simulating specific systems, engineering operations necessary for a scalable quantum information processing, or for developing new metrological devices. This ambitious scenario sets a rich, multidisciplinary environment ideal for generation of driving ideas, fast learning, technique sharing, and optimization of existing resources. The list of specific topics includes: cold chemical reactions, decoherence and measurement, entanglement, disordered potentials, operation engineering, optical lattices, quantum computation, quantum devices, quantum information, quantum metrology, quantum simulations, quantum statistical effects, shortcuts to adiabaticity, spin-orbit coupling, spintronics, tight-binding models, topological effects, trapped ions, ultracold atoms.

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RF & Microwave Group

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Department of Electricity and Electronics, Faculty of Science and Technology
University of the Basque Country

KEY WORDS: radio-frequency, microwaves, devices, circuits, systems, instrumentation, analysis

The *RF & Microwave Group* works in the field of high frequency devices, circuits and systems for different applications: wireless communications, radio navigation and scientific equipment. Their basic research axes are focused on the analysis and design of microwave circuits and high frequency instrumentation.

1. **Analysis and Noise Characterization of Microwave Power Amplifiers.** Amplifiers add noise to the desired signal producing degradation of sensitivity, resolution and signal quality in electronic systems. Amplitude Modulation (AM) and Phase- Modulation (PM) noise spectra measurement provide a complete picture of the amplifier noise behavior, including flicker and white noise contributions.
2. **Stability Analysis of Power Amplifiers for Satellite Applications.** Some techniques have been proposed and developed to check stability and to improve circuit design cycles, mainly focusing on high power solid-state amplifiers for satellite communications.
3. **Instrumentation at high frequencies.** Instrumentation for linear RF particle accelerator: beam position monitoring and generation and control of RF signals

Speech Interactive Research Group: Emotions and Dialogues

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KEY WORDS: speech technologies, spoken dialogue systems, emotions from speech, subjective language in internet, pattern recognition, machine learning.

The Speech Interactive Research Group (SPIN) focusses now on the detection and identification con emotional cues from speech signal as well on the detection and identification of subjective language forms, such as irony or sarcasm, on dialogic language on social web. We aim to understand the user, the semantic of the message emitted, the emotions involved in it, the intentionality of the content and the communicative goals of each user interacting with a machine. Thus the other main important research goal is the development of spoken dialog systems capable to deal with the user goals, as well as with the application or tasks goals and consider the user emotions and their evolution during the communication process. This communicational model has also to consider the history of the dialog and implement a natural and empathic dialog style.

To this end the group develops technologies based on data-driven approaches. In particular our contributions are based on stochastic finite-state automata, transducer and bi-automata whose parameters are estimated trough grammar inference algorithms and allow for machine composition as well as online adaptation to the user or to the task. Recently the group has also gone into technologies based on bi-LSTM and similar neural networks architectures to develop ASR and user models to train dialog managers. Moreover we are now dealing with end-to-end dialog generation using both stochastic bi-automata and bi-LSTM to manage the dialog.

The group participates in scientific projects granted by the National Spanish Minister for Science in collaboration with other outstanding research groups in Spain. We have also participated in international collaborations such as the eINTERFACE project in 2016. Currently we have a stable collaboration with the University of California-Santa Cruz to develop the SOFOCO corpus which consists of online debates and it is aimed at extracting cues for the identification of subjective language in Spanish. We also coordinates the project EMPATHIC (769872) H2020-SC1-2017-CNECT-1 just proposed to be granted by the European Commission.

Regarding knowledge transfer to the society we have now some research activities under contract with Vicomtech-IK4, a collaboration with e-Faber to develop a platform for scientific crowd-annotation and a stable collaboration with Intelligent Voice in the UK to develop ASR and SDS under neural network approaches

Theory of nanophotonics: Controlling light at the nanoscale with plasmonic nanoparticles

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KEY WORDS: plasmon, metal nanoparticle, nanoantenna, electromagnetic field, light

Thanks to the significant advances of fabrication techniques in the last decades, it is now possible to realize systems including nanosized components with a control of few tens of nanometers in size and geometry. This achievement has paved the way for the manipulation of light below the diffraction limits: indeed, metal nanoparticles are able to convert Visible-Near-Infrared light into collective excitations of conduction electrons at the nanoscale, called plasmons. At light wavelengths resonant with the plasmon, the metallic structures feature a remarkable absorption, despite their nanometric size, and an intense electromagnetic field enhancement and localization in proximity of their surface (accompanied by a notable temperature increase). For this reason metallic nanostructures are often referred to as nanoantennas.

Within this framework, we try to shed light on how to describe the phenomena taking place between nanoantennas separated by nanometric gaps. As a matter of fact, the plasmon-induced intense electromagnetic field is further enhanced in intermediate regions between antennas with nanometric separation, so called hot-spots. However, when the gaps are shrunk down to the nanometer, not only do other phenomena start to play a significant role (e.g., tunneling), but also the commonly used classical description does not hold any more and a quantum description is required [1].

The plasmon-excitation can also be exploited in combination with other optical effects. For instance, under the application of a static magnetic-field, magneto-optical (e.g., nickel) nanoantennas give rise to a component of the electric field in a direction orthogonal to the incident one. When the nanoantennas are placed in a periodic structure, the new component is not only enhanced due to the plasmon but also significantly modulated by the diffractive coupling introduced by the periodic arrangement [2].

Metal nanoantennas can also be effectively combined with phase-transition materials, such as materials whose optical properties change abruptly on a temperature basis (e.g., vanadium dioxide) [3]. Thanks to the plasmon-induced enhancement of the electromagnetic field it is possible to modulate down to the nanoscale the spatial temperature distribution in a phase-transition material, thus obtaining an all-optical active control of the material properties.

The theoretical study of this plasmonic light-matter interaction, spanning from the understanding of the key-mechanisms to the prediction of the induced phenomena, is of paramount importance for steering future efforts in the realization of effective electronic and optical nanodevices, such as molecular sensors, all-optical switches and thermal memristors.

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Digital Electronic Implementations for Computational Intelligence Applications

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KEY WORDS: digital electronics, system modelling, embedded systems, field-programmable gate arrays (FPGAs), computational intelligence, machine learning, data mining, intelligent environments, internet of things (IoT)

The Digital Electronics Design Group (GDED) focuses on two main lines of research aimed at the development of innovative multidisciplinary applications. These lines and their application areas are:

1. **Modelling of complex dynamic systems:** computational intelligence (neural networks, neuro-fuzzy systems, and genetic algorithms), optimization techniques, data mining, and machine learning for regression and multiclass classification problems.
2. **Design of efficient embedded electronic systems for real-time applications:** systems on a chip (SoCs), dynamic reconfiguration of FPGA devices, hardware/software co-design, high computational efficiency hardware accelerators, device consumption and size reduction techniques, "hardware-in-the-loop" co-simulation, and sensor technologies.
3. **Application areas:** ambient intelligence, intelligent agents on a chip, advanced driver assistance systems (ADAS), wireless sensor networks (WSN), environmental and physiological sensors, human activity recognition and wearable computing, internet of things (IoT), optimum and predictive controllers, and modelling and optimization of industrial processes (energy co-generation).

RECENT APPLICATIONS DEVELOPED BY THE GROUP AND WORK IN PROGRESS

The automotive industry is engaged in achieving the level "zero-accidents" and the autonomous driving. On the path to these top objectives, this sector demands highly enhanced driving assistance systems (DAS), where a huge amount of signals have to be processed in "real time" by means of very fast electronic systems. The group has reported the development of an embedded electronic system aimed to improving driver safety, security, and well-being in a non-intrusive manner. Present objectives of GDED in this line include the design of new hardware/software platforms, based on machine learning intellectual property (IP) cores, that are capable of recognizing driver states, as drowsiness and alert loss, which will enhance vehicle safety and reliability.

On the other hand, Ambient Intelligence proposes a model where people are assisted by an invisible and ubiquitous electronic environment. Intelligent agents have to process a huge amount of signals coming from multiple sensors, and they have to be capable of responding in real-time. The group has developed an autonomous single-chip electronic system, based on FPGA, suitable for integration in a network of cooperative devices.

In addition, the group has participated in an industrial project oriented to improve efficiency in a cogeneration plant, as well as in other designs in the context of wearable computing and human activity recognition (HAR).

In all these application areas the group works on approaches that process very large and complex data sets and often respond in real-time, by taking advantage of data mining techniques, computational intelligence solutions, machine learning algorithms, and advanced optimization strategies.

GEOLOGÍA



Geobiodiversity: Geology, Fossil record and Heritage from the Mesozoic and Cenozoic of the Western Pyrenees

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KEY WORDS: biodiversity, vertebrates, geology, Mesozoic, Cenozoic, Western Pyrenees, palaeontological heritage.

The Geobiodiversity research group (IT 1044-16 of the Basque University System) includes geologists and palaeontologists from the Universidad del País Vasco/Euskal Herriko Unibertsitatea (UPV/EHU), in collaboration with researchers from other centers and institutions (i.e., museums and universities), both national and foreign.

The main objective of our research is to contribute to the better knowledge of the palaeodiversity of the Western Pyrenees from the study of the fossil record of continental and marine vertebrates and associated biota from the Mesozoic and Cenozoic of the Basque-Cantabrian Region and adjacent basins. The fossil record, as a part of the geological record, is a non-renewable historical archive and constitutes the main tool for the study of the biodiversity of the past and of the biosphere evolution. This is directly related to the geological processes that have occurred throughout the history of the Earth.

Main lines of research:

1. Mesozoic and Cenozoic vertebrate faunas and associated biota of the Western Pyrenees: Taphonomy, Paleobiology, Geology and Geochronology.
2. Synsedimentary tectonics, hydrothermalism and biotic changes in Cretaceous seas.
3. Human evolution and palaeoecology of the Quaternary.
4. Geodiversity and palaeontological heritage.

The activities of the research group can be summarized into three: A) Research; B) Dissemination of scientific and educational findings; and C) Geoconservation.

Recent publications:

- Astibia H., Badiola A., Bardet N., Berreteaga A., Corral J.C., Díez Díaz V., Elorza J., Ortiz S., Payros A. & Pereda Suberbiola X. (2013). El Registro fósil de los Pirineos Occidentales: estudio, importancia y gestión de un gran archivo de paleobiodiversidad. *Euskonews*, 673. <http://www.euskonews.com/0673zbk/gaia67303es.html>

- Badiola A., Pereda-Suberbiola X., Astibia H., Bardet N., Berreteaga A., Bodego A., Corral J.C., Díaz-Berenguer E., Díaz-Martínez I., Díez Díaz V., Elorza J. & López-Horgue M. (2015). Paleobiodiversidad de vertebrados de los Pirineos Occidentales: yacimientos de interés patrimonial en la Región Vasco-Cantábrica y áreas adyacentes (Cretácico-Neógeno). *Cuadernos del Museo Geominero*, 18: 113-118.

- Bodego A., López-Horgue M., Astibia H., Badiola A., Berreteaga A., Corral J.C., Martínez-García B., Ortiz S., Pereda Suberbiola X., Rofes J. & Suarez-Hernando O. (2014). Registro fósil de la Región Vasco-Cantábrica y áreas adyacentes de los Pirineos Occidentales. En: *Geología de la Cuenca Vasco-Cantábrica*, Servicio Editorial de la UPV/EHU, pp. 141-155. Also Basque version (2014) in *Euskokantauriar Arroko Geologia* (Bodego et al., Eds.).

Contribution to habitat and socio-economic knowledge of (pre-)historic epochs from the archaeological records

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KEY WORDS: C isotope, N isotope, Sr isotope; O isotope, archaeological materials, bones, teeth, gastropods, slags, mortars, pottery.

Multi-disciplinary research group formed by geologists, archaeologists and anthropologists investigate habit and socio-economics evolution of (pre-)historic epoch from archaeological records. Research team integrates senior and junior members that have been collaborating during several years. Two main research lines according to the studied material are developed in the archaeometric field.

1. **Fossil remains** allow reconstructing climatic and environmental conditions during the last 100 or 120 thousand years. On the other hand, by means of isotope composition diet and migrations patterns of ancient human and fauna can be established.
2. **Archaeological materials** provides clues of human technological evolution, technological skills, and cultural and trade links.

PALAEOCLIMATIC AND PALAEOENVIRONMENTAL RECONSTRUCTION

Variability in climate and local environment determines food source availability, and different food sources have particular stable carbon and nitrogen isotope values. Since the food isotopic signal is reflected in bone collagen and teeth, this can be used as a proxy to infer palaeodietary and palaeoclimatic variations.

The stable carbon isotope ratio ($\delta^{13}\text{C}$) of human and fauna tissue is related to factors such as the environment, the photosynthetic pathways of consumed plant matter, humidity, water availability, salinity, and partial atmospheric $p\text{CO}_2$. By contrast, nitrogen isotope ratios ($\delta^{15}\text{N}$) preserved in tissues are related to factors such as diet, climate, and water availability. Some of the studied cases can be found in: Rofes et al. (2015) *Scientific Reports* 5, 1-12. Castaños et al. (2014) *Quaternary International* 339-340, 131-138.

PALAEODIETARY AND MOBILITY PATTERNS OF HUMAN POPULATIONS

On the other hand the analysis of carbon and nitrogen isotope composition in human bone collagen constitutes an approach to palaeodietary reconstruction and provide information about the protein portion of the diet averaged over at least the last 10 years prior to death and also about different protein sources.

Strontium and oxygen isotopes are used to identify migrants and to reconstruct movements of past populations. Both isotopes are two independent isotopic systems in which strontium reflects local geology and oxygen reflects geography. Some cases studied by our team correspond to: Ortega et al. (2013) *Quaternary International* 303, 54-63. Guede et al. (2015) *Metrology for Archaeology*, 413-418.

HUMAN TECHNOLOGICAL EVOLUTION

Archaeometric researches are performed on archaeological pottery, lime mortars and historical slags among others. Technique variations between communities and temporal evolution of technologies are valuable topics to get a comprehensive knowledge of social evolution along time. Some case studied can be found in: Zuluaga et al (2012) *J. Raman Spectrosc.* 43, 1811-1816; Portillo et al (2016) *Geogaceta*, 60, 115-118.

Global Boundary Stratotype Section and Points (GSSPs) in the Basque Coast

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KEY WORDS: Paleogene, Stratigraphy, Geological Time Scale

The Geological Time Scale is a valid global frame divided into intervals (Eons, Eras, Periods, Epochs and Stages) whose definition is based primarily on Stratigraphy. The International Commission on Stratigraphy (ICS) is responsible for selecting the geological sections worldwide that best represent the boundaries between unit intervals. Stage boundaries are defined by Global Stratotype Sections and Points (GSSPs). The *Cretaceous and Paleogene working Group* (Research Group IT-631-13) of the Faculty of Science and Technology has organized several international meetings in 2006, 2007 and 2009, which showed the International community, and ultimately the ICS, the high geological quality of the Basque coastal cliff sections. These are now a worldwide reference to observe and study the sedimentary rocks accumulated in deep-marine settings from the Early Cretaceous to the Eocene, a lapse interspersed with some of the most significant global change events. As a result, the Itzurun beach at Zumaia (Gipuzkoa) was selected for the GSSP for the Selandian and Thanetian stages and the Gorronatxe Beach (Bizkaia) for the GSSP of the Lutetian stage.

The GSSPs for the bases of the Selandian and Thanetian stages

In the hemipelagic section exposed at Zumaia the base of the Selandian Stage has been placed at the base of the Itzurun Formation, ca. 49 m above the Cretaceous/Paleogene boundary. At the base of the Selandian, marls replace the succession of Danian red limestone-marl alternation. The global correlation criterion for the basal Selandian is the second radiation of an important calcareous nannofossil group, the fasciculiths. Species such as *Fasciculithus ulii*, *F. billii*, *F. janii*, *F. involutus*, *F. pileatus* and *F. tympaniformis* have their first appearance in the interval from a few decimetres below up to 1.1 m above the base of the Selandian. The marker species for nannofossil Zone NP5, *F. tympaniformis*, first occurs 1.1m above the Selandian GSSP. Excellent cyclostratigraphy and magnetostratigraphy in the section creates further correlation potential, with the base of the Selandian occurring 30 precession cycles (630 kyr) above the top of magnetochron C27n. Profound changes in sedimentology related to a major sea-level fall characterize the Danian-Selandian transition in sections along the margins of the North Atlantic. The base of the Thanetian Stage is placed ca. 78m above the Cretaceous/Paleogene boundary. It is defined at a level 2.8m or eight precession cycles above the base of the Mid-Paleocene Biotic Event, and is located at the base of magnetochron C26n. The base of the Thanetian is not associated with any significant change in marine micro-fauna or flora. The calcareous nannofossil Zone NP6, marked by the first occurrence of *Heliolithus kleinpelli* starts ca. 6.5 m below the base of the Thanetian. The definitions of the global stratotype points for the bases of the Selandian and Thanetian stages are in good agreements with the historical stratotype sections defined in Denmark and England, respectively.

The GSSP for the base of the Lutetian Stage.

The GSSP for the base of the Lutetian Stage (early/ middle Eocene boundary) is defined at 167.85 metres in the Gorronatxe sea-cliff section (NW of Bilbao city, Basque Country, northern Spain; 43°22'46.47" N, 3° 00' 51.61" W). This dark marly level coincides with the lowest occurrence of the calcareous nannofossil *Blackites inflatus* (CP12a/b boundary), is in the middle of polarity Chron C21r, and has been interpreted as the maximum flooding surface of a depositional sequence that may be global in extent. The GSSP age is approximately 800 kyr (39 precession cycles) younger than the beginning of polarity Chron C21r, or -47.8 Ma in the GTS04 time scale. The proposal was approved by the International Subcommission on Paleogene Stratigraphy in February 2010, approved by the ICS in January 2011, and ratified by the International Union of Geological Sciences (IUGS) in April 2011.

Cenozoic fossil record study

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KEY WORDS: Cenozoic, fossil record, research team, divulgation.

Our research team works in the study, protection and diffusion of the fossil record from Miocene to Holocene, covering the last 23 million years of the Earth. The fossil remains that we study were produced by organisms which lived in continental environments. In particular, we study the taxonomy, biodiversity and ecological meaning of vertebrates, ostracods and charophytes, because they are the best preserved fossils. Due to this kind of studies, we can reconstruct the climate and the environment conditions to each stratigraphic unit. In this way, if we make this study in the all levels of one site, we can infer the palaeoenvironmental reconstruction over the time to this area. In addition, a lot of climate changes and organisms extinctions have been occurred throughout geological history. So, both the palaeoenvironment reconstructions and the presence or/and absence of an specific taxon allow us to deduce about a relative dating. Specifically, our group study most of the quaternary deposits from the Cantabrian Region and also the miocene sites from the northwest Sector of the Ebro Basin, comprising more than 30 sites.

Scientifically these types of studies are very important, but transmit and make these results public it is very interesting and essential too. For that reason, all the members of our group take part in numerous activities of divulgation which are related to Geology. Amongst them, we can stand out the field trips with secondary school students, the organization of activities for the Week of Science, the planning of Geodays, the visits to primary and secondary schools, the guided visits into the University of the Basque Country, the impartation of conferences...

Behaviour of B, Li, P and other rare-elements in crustal materials during the Variscan Orogeny

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KEY WORDS: Variscan orogeny, pegmatites, tourmaline, boron, lithium, phosphorous.

Research lines:

1. **Rare-element pegmatites** (mainly rich in Li and Sn, but also enriched in Nb-Ta, Rb, Cs, B, F and P in many cases) are common in the Central Iberian Zone (CIZ) (Spain and Portugal). These pegmatitic bodies show not only a high scientific interest, but also an important economic interest, when elements and minerals associated with pegmatites are being more and more demanded by the new technologies. We are developing a global study of the pegmatites from this area, in order to obtain a valuable information not only on the geology of the pegmatites themselves, but also on the regional geology and on the geochemical behaviour of some elements (e. g. P, B, F, Li, Rb, Sn, Nb, Ta among others) during pegmatitic crystallization. The better knowledge of the mineralogical and petrogenetical features of these rocks would facilitate the knowledge and understanding of the anatomy and regional distribution of pegmatites, which is definitively helpful for the exploration and exploitation of the important mineral resources frequently found associated to the pegmatitic rocks.
2. **Tourmaline bearing rocks** are also common and even locally abundant in the CIZ. The occurrence of tourmaline in different lithologies of this area suggests that B played an important roll during the Variscan orogeny. This way, a good knowledge on the source of B, the processes that favoured the tourmalinization events, the possible recycling of boron from tourmaline-rich pre-Variscan rocks, and the evolution and distribution of B during the Variscan cycle, will help in the understanding of the whole Variscan orogeny.

RESEARCH PROJECTS DURING THE LAST FIVE YEARS

- Reciclaje de boro y formación de turmalina en el complejo del Álamo (Zona Centro Ibérica, España): implicaciones geológicas.
- Grupo de investigación del comportamiento del B, Li, P y otros elementos raros en materiales corticales durante la orogenia Varisca.
- Distribución y comportamiento del litio y otros elementos asociados en el orógeno herciniano de la CIZ.
- Mineralizaciones de litio asociadas a pegmatitas de la Península Ibérica.

COOPERATION WITH OTHER INSTITUTIONS

- Lab. Minéralogie et Cristallographie, Univ. Paul Sabatier, Toulouse, (France)
- Institut für Mineralogie und Kristallchemie, Univ. Stuttgart, (Germany)
- Lab. Cristallographie et Minéralogie, Univ. Lieja, (Belgium)
- Faculdade de Ciencias, Universidade do Porto, (Portugal)
- Consejo Nacional de Investigaciones Científicas y Técnicas, (Argentina)
- Universidad de Calcuta (India)
- University of New Orleans and MP2 (Mineralogy & petrology of Pegmatites)
- Maine Mineral & Gem Museum,
- Department of Mineralogy from the Natural History Museum de Oslo, Noruega.

OTHER ZONES OF RESEARCH

- Pegmatites from the San Luis Range (Argentina)
- Pegmatites from New Hampshire and Maine States (USA)

HAREA-Coastal Geology Research Group

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KEY WORDS: environmental transformation, natural processes, anthropogenic impact

The Harea-Coastal Geology research group (www.ehu.eus/harea-geologicalitoral) develops a multidisciplinary approach (sedimentology, geochemistry, micropalaeontology, topography, radiometric chronology) to characterize natural and anthropogenic processes responsible for the environmental transformation of the coastal zone during the last climate cycle (Holocene and Anthropocene). Its activities can be summarized into the following research lines and recent publications:

1. **Environmental transformation of polluted and regenerated ecosystems.** The coastal area has experienced an intense human pressure that provoked its physical destruction and a deep chemical and biological transformation. The development of environmental conservation and regeneration schemes makes necessary to carry out geological studies to evaluate their modern characteristics, historical alteration processes and the feasibility of improvement proposals (Leorri, E.; Mitra, S.; Irabien, M.J.; Zimmerman, R.; Blake, W.H. and Cearreta, A. (2014). 700 yr record of combustion-derived pollution in northern Spain: tools to identify the Holocene/Anthropocene transition in coastal environments. *Science of the Total Environment* 470-471: 240-247).
2. **Sea-level variations as a consequence of anthropogenic climate change.** An increase in sea-level rise rate is potentially one of the most devastating impacts of the future climate change on coastal areas. Climate change influences the coastline at decadal and centennial scales, and these variations of the relative sea level are registered in the coastal sedimentary sequences. The combined study of historical records and high resolution geological reconstructions of the relative sea level is a powerful tool (García-Artola, A.; Cearreta, A.; Irabien, M.J.; Leorri, E.; Sanchez-Cabeza, J.A. and Corbett, D.R. (2016). Agricultural fingerprints in salt-marsh sediments and adaptation to sea-level rise in the eastern Cantabrian coast (N. Spain). *Estuarine, Coastal and Shelf Science* 171: 66-76).
3. **Holocene environmental evolution due to natural processes.** Due to the frequent, rapid and intense climate changes that characterize the late Quaternary, coastal environments have experienced dramatic variations and contain a complete record of the processes and events occurred during this interval. The high-resolution multiproxy study of the sedimentary record allows reconstruction of the past features, to understand the present conditions and to deduce the future environmental variability (García-Artola, A.; Cearreta, A. and Leorri, E. (2015). Relative sea-level changes in the Basque Coast (northern Spain, Bay of Biscay) during the Holocene and Anthropocene: the Urdaibai estuary. *Quaternary International* 364: 172-180).
4. **Sedimentary processes with social and economic consequences.** Sedimentary processes in the estuarine areas are frequently altered by human-induced activities (dredgings, dumpings, reclamation, channeling) which can lead to undesirable repercussions. Sedimentological studies contribute to understand the role of the anthropogenic influence and to establish suitable strategies for sustainable development (Leorri, E.; Cearreta, A.; Irabien, M.J.; García-Artola, A.; Corbett, R.; Horsman, E.; Blake, W.H. and Sánchez-Cabeza, J.A. (2014). Anthropogenic disruption of the sedimentary record in coastal marshes: examples from the southern Bay of Biscay. *Continental Shelf Research* 29: 1226-1239).
5. **Anthropocene: a new epoch in the geological scale?** Human activity is leaving a pervasive and persistent signature on Earth. Numerous anthropogenic markers of functional changes in the earth system have been found through the stratigraphic record. These signals render the Anthropocene stratigraphically distinct from the Holocene (Waters, C.N.; Zalasiewicz, J.; Summerhayes, C.; Barnosky, A.D.; Poirier, C.; Gałuszka, A.; Cearreta, A.; et al. (2016). The Anthropocene is functionally and stratigraphically distinct from the Holocene. *Science* 351 (6269): aad2622.1-aad2622.10).

This research group has a leading role in the Postgraduate Programmes (Master and Doctorate) and the UFI on Quaternary: Environmental Changes and Human Footprint (www.ehu.eus/mastercuaternario, www.ehu.eus/doctoradocuaternario, www.ehu.eus/uficuaternario). Acknowledgements: IT767-13 (Basque Government) and UFI 11/09 (UPV/EHU).

Development of SOFC components

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KEY WORDS: combustion synthesis, SOFC components, SOFC commercialization.

ABSTRACT

Solid oxide fuel cells (SOFCs) have the potential to be one of the cleanest and most efficient energy technologies for direct conversion of chemical fuels to electricity. Economically competitive SOFC systems appear poised for commercialization, but widespread market penetration will require continuous innovation of materials and fabrication processes to enhance system lifetime and reduce cost. Additional requirements arise for the technologies for synthesis of SOFC materials. These requirements originate from the demands for large scale SOFC industrial production. In this sense, solution combustion synthesis (SCS) is a simple and reproducible method used to obtain several types of ceramic oxides for a variety of applications. A typical SCS procedure utilizes a self-sustained exothermic reaction among well-mixed reactants to achieve the rapid and economical synthesis of particulate products. Up to 2008, SCS method has been adopted to fabricate more than 1000 kinds of oxide powders over more than 65 countries [1]. The properties of the resulting powders (crystalline structure, amorphous structure, crystallite size, purity, specific surface area and particle agglomeration) depend heavily on the adopted processing parameters [2,3].

For these reason, we have synthesized different parts of a fuel cell, on a large scale, by the glycine-nitrate combustion method. It have been synthesized interconnector protective coatings ($\text{MnCo}_{1.9}\text{Fe}_{0.1}\text{O}_4$), contact layers ($\text{LaNi}_{0.6}\text{Fe}_{0.4}\text{O}_3$), cathodes ($\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_3$), interlayers ($\text{Sm}_{0.2}\text{Ce}_{0.8}\text{O}_{1.9}$), electrolytes ($\text{ZrO}_2)_{0.92}(\text{Y}_2\text{O}_3)_{0.08}$ and anode ($\text{Ni}_{0.3}\text{O}-(\text{ZrO}_2)_{0.92}(\text{Y}_2\text{O}_3)_{0.08}$) materials, obtaining reproducible pure samples and amounts up to 12 g for each batch, being able to increase easily this amount to lots of hundred of grams. The obtained materials have been characterized compositionally by inductively coupled plasma atomic emission spectroscopy (ICP-AES) and X-ray fluorescence (XRF), structurally by X-ray diffraction (XRD), microstructurally by scanning electron microscopy (SEM) and by conductivity measurements.

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MATEMÁTICAS



Effective time-domain goal-oriented adaptive algorithms

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KEY WORDS: wave equation, goal-oriented adaptivity, error representation, Finite Element Method.

Goal-oriented adaptive algorithms [2,4] have been widely employed during the last three decades to produce optimal grids in order to solve challenging engineering problems. In this work, we extend the theory developed in [3] in the context of frequency-domain wave-propagation problems, to the case of time-domain problems. In the aforementioned work, unconventional dual problems are used in order to define an error representation and perform goal-oriented adaptivity. To do that, we express the entire problem in weak form [1] to formulate the adjoint problem and apply the goal-oriented adaptivity [5]. Some numerical results are provided in 1D which show that the upper bounds of the new error representation are sharper than the classical ones and therefore this new error representation can be used to design goal-oriented adaptive processes.

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Comparison of some methods with numerical dissipation when solving the wave equation

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KEY WORDS: wave equation, Finite Element Method, numerical dissipation, stiff ODEs.

The one-dimensional linear wave equation with boundary conditions (BC) and initial conditions (IC) in a string of length L has been considered. Let $u(x,t)$ denote the vertical displacement of the string from the x axis in time t . It is assumed that the string is undergoing small amplitude transverse vibrations so that $u(x,t)$ obeys the wave equation. This equation has been discretized using the Finite Element Method (FEM) [2, 6, 7] using linear and quadratic shape functions, obtaining a stiff system of second order Ordinary Differential Equations (ODEs) [3]. The high-modes of the resulting ODE system are consequence of the FEM approximation and they are not representative, so they have to be removed from the solution to avoid inconvenient noise [1]. Solving stiff ODEs requires the use of numerical methods with good stability properties and controlled numerical dissipation in the high-frequency range. The HHT- α and the Collocation methods are second order precision, unconditionally stable and able to dissipate high-modes for some values of the parameters [4, 5]. They both operate directly in second order ODEs. We have calculated the parameters for which the numerical dissipation of these methods in the high-frequency range is similar. We have solved the wave equation obtaining noise free and accurate solutions.

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Matrix analysis and applications group

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KEY WORDS: matrix analysis, control theory, linear systems, structure invariants, perturbation, numerical linear algebra, inverse problems, canonical forms, eigenvalues, singular values.

The Group of Matrix Analysis and Applications (GAMA) of the University of the Basque Country is the result of the evolution of a team that has been working uninterrupted in research since 1981. The main research areas of this group are:

- Theory of matrices.
- Mathematical control theory.
- Perturbation theory.
- Numerical linear algebra.

The aim of our research is to gain insight into the structure of the linear control systems and matrices and to develop mathematical techniques in order to solve problems in these areas. The following research lines have been designed:

- Study of the structure of control systems and matrices.
- Spectral perturbation of matrices and linear systems.

These research lines are closely related. Nevertheless, in order to clarify the problems that we are interested in, we will state, in a general manner, some of them:

1. Pole assignment to singular systems by state feedback and output injection.
2. Obtain an explicit versal deformation of a controllable and observable system and translate it to the perturbations of the corresponding finite sequence of Markov parameters.
3. Characterize the matrices that are coprime at infinity and provide, by local techniques, conditions for the strong equivalence of matrix polynomials.
4. Give necessary and sufficient conditions for the existence of symmetric quadratic matrix polynomials with positive (semi)definite coefficients and prescribed eigenvalues. Give a procedure to construct wide families of such matrices.
5. Give a complete description of the behavior of the A5/1 algorithm and understand it in a theoretical context.
6. Study the change of the controllability indices of a controllable pair when the elements of a column of the control matrix are slightly perturbed.
7. Obtain a canonical form for the left (m_1, m_2) -Wiener-Hopf equivalence at infinity.
8. Analyse the geometry of the pseudospectrum connected components and find its derivatives in the Hausdorff metric sense.
9. Find the distance, in the spectral norm, from a matrix to the set of matrices that have prescribed one eigenvalue and a partition which lowerly bounds the Weyr's partition of this eigenvalue for the order of weak majorization.

The methods and techniques to be used run over almost all fields of mathematics: from Linear Algebra and Matrix Analysis or Combinatorics to Differential Geometry or Commutative Algebra.

Weekly seminars are kept where the progression of the subgroup's work is shown, the difficulties are discussed and other researchers' work related to our problems is explained. This and the individual study of papers are the main methodological tools. The results are published in the most important specialised journals: Linear Algebra and its Applications, SIAM Journal of Control and Optimization, SIAM Journal on Matrix Analysis and Applications, International Journal of Control, Linear and Multilinear Algebra, Electronic Journal of Linear Algebra, etc.

More information in: <http://www.ehu.eus/gama>

Biostatistics Research Group

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KEY WORDS: Biostatistics; Clinical research; Transfer

The main specific objectives of the group are to detect problems of scientific interest in the biomedical and experimental fields where biostatistics can contribute to their resolution; conduct our own research in biostatistics aimed at generating results for solving the problems; create necessary computer tools and software for its implementation; and apply the proposed methods to the considered problems, helping to interpret the results and draw final conclusions, in collaboration with biomedical and experimental researchers involved.

Other objectives of the group are basically transversal, such as, to give methodological support in biostatistics to other research groups in the fields of biomedicine or experimental sciences; to promote the transfer of the research done at the university in biostatistics to biomedical and experimental fields; to take advantage of the strong demand for support in biostatistics to detect future research in this area, that respond to real problems in other fields.

NEW RESEARCH LINES:

1. **Development of an overall score of evaluation from the responses to a questionnaire by MCA.** The aim of this work is to propose a method for developing a summary score based on the answers from a questionnaire where a one dimensional structure is confirmed and all the variables modalities are sorted in the first dimension from the MCA.
2. **Development and validation of statistical tools for handling longitudinal missing outcomes.** Missing data are a common problem among various types of medical design studies. It is especially problematic in longitudinal studies that require repeated measures, in which the missingness rates can become high and relevant. The main goal of this study is to develop and validate statistical approaches for Health Related Quality of Life (HRQoL) longitudinal missing outcomes when non-ignorability is present.
3. **Comparison of beta-binomial regression model approaches to analyze HRQoL data.** Beta-binomial distribution has been shown to be an adequate distribution to fit HRQoL data in the literature. The aim of this work is to compare in terms of covariate effect the existing regression approaches based on the beta-binomial distribution.

KNOWLEDGE TRANSFER:

- **Implementation of predictive models in technological tools.** We have developed a valid and reliable computer tool (PREVEPOC) for the assessment of the severity of a patient with chronic obstructive pulmonary disease (COPD). It allows to estimate quickly the risk of evolution in patients who come to emergency departments with an COPD.
- **Software Development.** We are working on the implementation of the methodology developed in this group into R or SAS packages.
 - CatPredi an R package to categorize continuous variables in prediction models.
 - HRQoL is an R package to develop analysis related with HRQoL data; such as specific recodes, plots and models. Available at <https://github.com/idaejin/HRQoL>
 - ZScore an R package to develop an overall score of a questionnaire responses by MCA.
 - Statistical Simulation Performance (SSP) a statistical toolkit composed by an R package, SAS@ macro and a web application to assess the performance of the obtained simulation results.

FOR MORE INFORMATION LOOK AT THE FOLLOWING WEB PAGE <https://sites.google.com/site/biostit/>

Mathematical Analysis: Mathematical Physics

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Discrete Uncertainty Principles

• Classical Uncertainty Principles

The classical Hardy and Heisenberg uncertainty principles assert that a function and its Fourier transform cannot be simultaneously localized.

• Discrete Uncertainty Principles

We are currently working on versions of these results in a discrete setting, where we consider a discrete spatial variable $k \in \mathbb{Z}$ and we replace the usual Fourier transform by the so called discrete-time Fourier transform. Real-variable techniques similar to those used in [1] lead to:

Theorem 1 ([2, 3]) Let u be a solution to

$$\partial_t u(k, t) = i[u(k+1, t) - 2u(k, t) + u(k-1, t)] + V(k)u(k, t)$$

in $\mathbb{Z} \times [0, 1]$ with $V \in L^\infty$. There exists $\mu_0 > 0$ such that if $\mu > \mu_0$ and

$$\sum_{k \in \mathbb{Z}} e^{2\mu|k| \log|k|} (|u(k, 0)|^2 + |u(k, 1)|^2) < +\infty;$$

then, $u \equiv 0$. Hence, a solution to the discrete Schrödinger equation cannot have fast decay at two different times.

The decay assumed for the solution at times $t = 0$ and $t = 1$ in Theorem 1 is related to the modified Bessel function I_k , as it happens in the continuous case with the Gaussian [1].

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Borderline weighted estimates for commutators

• Averages and maximal operators

Given a strictly increasing and convex function A such that $A(0) = 0$ and $A(t) \rightarrow \infty$ as $t \rightarrow \infty$, we define the average of f with respect to A over a cube Q as

$$\|f\|_{A(L), Q} = \inf \left\{ \lambda > 0 : \frac{1}{|Q|} \int_Q A \left(\frac{|f(x)|}{\lambda} \right) dx \leq 1 \right\}.$$

We can define maximal operators related to those averages as follows

$$M_{A(L)} f(x) = \sup_{x \in Q} \|f\|_{A(L), Q}.$$

If $A(t) = t \log(e+t)^\rho$ for $\rho > 0$ we denote $M_{A(L)} = M_{L(\log L)^\rho}$. Similarly if $A(t) = t \log(e+t) \log(e+\log(e+t))^\rho$ for $\rho > 0$, we write $M_{A(L)} = M_{L \log L(\log \log L)^\rho}$.

• Borderline weighted estimates for commutators

Given $b \in BMO$ and T a Calderón-Zygmund operator we define the commutator $[b, T]$ as

$$[b, T]f(x) = b(x)Tf(x) - T(bf)(x).$$

We have obtained the following quantitative estimate [3]:

$$w_{[b, T]f}(\lambda) \lesssim \frac{1}{\varepsilon^2} \int_{\mathbb{R}^n} \Phi \left(\frac{\|b\|_{BMO} |f(x)|}{\lambda} \right) M_{L \log L(\log \log L)^{1+\varepsilon}} w(x) dx \quad \varepsilon > 0,$$

where $w_{[b, T]f}(\lambda) = w(\{x \in \mathbb{R}^n : |[b, T]f(x)| > \lambda\})$ and $\Phi(t) = t \log(e+t)$. This estimate is a quantitative version of the main result in [2] and it is also a natural counterpart to the quantitative estimate obtained in [1] for Calderón-Zygmund operators.

• Open questions

It should be possible to replace the maximal operator on the right hand side of the inequality by a smaller operator. For instance we should be able to obtain the following estimate

$$w_{[b, T]f}(\lambda) \lesssim \frac{1}{\varepsilon^2} \int_{\mathbb{R}^n} \Phi \left(\frac{\|b\|_{BMO} |f(x)|}{\lambda} \right) M_{L \log L(\log \log L)^{1+\varepsilon}} w(x) dx \quad \varepsilon > 0.$$

We also wonder whether the quadratic decay on ε is the best possible or if we could obtain a linear decay instead. That linear decay would lead to a better dependence on the A_1 constant in the case $w \in A_1$.

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Research Projects

IT641-13 (Gobierno Vasco, Grupos de Investigación), researcher in charge: Luis Vega. MTM2014-53145-P (Ministerio de Economía y Competitividad) researchers in charge: Luis Vega (1), Carlota Cuesta (2). MTM2014-53850-P (Ministerio de Economía y Competitividad) researchers in charge: Carlos Pérez (1), J.B. Bru (2). HADE-Harmonic Analysis and Differential Equations: new challenges (ERC-EA European Research Council Executive Agency), researcher in charge: Luis Vega.

Relativistic Quantum Mechanics

• Shell interactions for Dirac operators

The free Dirac operator is a first-order differential operator defined by:

$$H = -i\alpha \cdot \nabla + m\beta = \begin{pmatrix} m & 0 & -i\partial_3 & -\partial_2 - i\partial_1 \\ 0 & m & \partial_2 - i\partial_1 & i\partial_3 \\ -i\partial_3 & -\partial_2 - i\partial_1 & -m & 0 \\ \partial_2 - i\partial_1 & i\partial_3 & 0 & -m \end{pmatrix}.$$

The free Dirac operator is a first order differential operator satisfying $H^2 = (-\Delta + m^2)\mathbb{I}_4$ and governs the quantum relativistic dynamics of an electron of mass m with no external forces acting on it.

We study the shell interaction of measure valued potentials: let $\Omega \subset \mathbb{R}^3$ be a bounded regular domain, then we consider potentials V living at the boundary $\partial\Omega$ of Ω , i.e., V are $L^2(\sigma)^4$ -valued potentials, where σ is the surface measure of $\partial\Omega$.

For such potentials, in [1] we construct a domain of self-adjointness $D(H+V) \subset L^2(\mathbb{R}^3)^4$. In particular, we study Electrostatic plus Lorentz scalar potentials

$$V_{es}(\varphi) = \frac{1}{2}(\lambda_e + \lambda_s \beta)(\varphi_+ + \varphi_-), \quad \lambda_e, \lambda_s \in \mathbb{R} \text{ such that } \lambda_e^2 - \lambda_s^2 \neq 0, 4,$$

where φ_\pm are non-tangential boundary values of φ on $\partial\Omega$. We prove that $H + V_{es}$ defined on $D(H + V_{es})$ is self-adjoint and

- If $|\lambda_e| \notin [1/C, 4C]$ for some C that depends only on the surface ($\lambda_s = 0$), then $H + V_{es}$ has no eigenvalues in $(-m, m)$.

• Confinement

A potential V generates confinement with respect to H and $\partial\Omega$ if the particles under consideration which are initially confined in Ω at time $t = 0$ remain in Ω for all $t \in \mathbb{R}$ under the evolution $\partial_t = -i(H + V)$, i.e., $H + V$ makes $\partial\Omega$ impenetrable for particles.

In [1] we prove that V_{es} generates confinement w.r.t. H and $\partial\Omega \Leftrightarrow \lambda_e^2 - \lambda_s^2 = -4$, which extends previous results in [2].

• Current research

The MIT bag model is one of the simplest relativistic models for the confinement of an electron in a box, which is a particular case of the above-mentioned confinement potentials. Continuing with the work in [3] we want to study the eigenvalue problem for this model,

$$\begin{cases} H\psi = a\psi, & \text{in } \Omega \\ -i\beta(\alpha \cdot n)\psi = \psi, & \text{in } \partial\Omega \end{cases}$$

where $\psi \in H^1(\Omega)^4$, $a > 0$ and n is the exterior normal vector. We are interested in self-adjointness, spectral properties and the non-relativistic limit.

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Analytic parabolic equations and Control Theory

• Second order analytic parabolic equations: we consider the parabolic evolution

$$\begin{cases} \partial_t u - \sum_{i,j=1}^n a^{ij}(x, t) \partial_{x_i x_j} u = 0, & \text{in } \Omega \times (0, T] \\ u(x, t) = 0, & \text{on } \partial\Omega \times (0, T] \\ u(x, 0) = u_0, & u_0 \in L^2(\Omega). \end{cases} \quad (1)$$

We assume that the space-time dependent coefficients satisfy

- i) uniform parabolicity: for some $\lambda > 0$

$$\sum_{j,i=1}^n a^{ij}(x, t) \xi_i \xi_j \geq \lambda |\xi|^2 \quad \text{for } (x, t) \in \Omega \times (0, T], \quad \forall \xi \in \mathbb{R}^n;$$

- ii) real-analyticity: there exists $\rho_0 > 0$ such that

$$|\partial_x^\alpha \partial_t^k a(x, t)| \leq \rho_0^{-|\alpha| - k} |\alpha|! k! \quad \text{for } (x, t) \in \Omega \times (0, T] \text{ and } (\alpha, k) \in \mathbb{N}^n \times \mathbb{N}.$$

• Quantitative estimates of real-analyticity

Assuming that the boundary of the domain Ω can be described locally as the graph of a real-analytic function we have proved [2, 3] that solutions to (1) satisfy the following quantitative estimate of analyticity:

$$|\partial_x^\alpha \partial_t^k u(x, t)| \leq e^{\frac{\rho}{t}} \rho^{-|\alpha| - k} t^{-k} |\alpha|! k! \|u_0\|_{L^2(\Omega)} \quad (2)$$

with $(x, t) \in \Omega \times (0, T]$ and $(\alpha, k) \in \mathbb{N}^n \times \mathbb{N}$. Here ρ is a constant depending on ρ_0 and the real-analyticity of the domain Ω .

• Control Theory

The results obtained in [2, 3] are extensions of those in [1], where the estimate (2) is used to prove a null-controllability property from measurable sets for the Heat equation. In [3] we have extended the analyticity and controllability results to higher-order parabolic equations.

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Groups, Topology and Applications

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KEY WORDS: group theory, pointfree topology.

There is a strong trend of making mathematics more and more interdisciplinary. Often, it is at the frontier of two different branches of mathematics, where we see new ideas resolve long-standing problems. Our research group, *Groups, Topology and Applications*, as its name suggests covers two areas of basic research, Group Theory and Topology and seeks to explore their interactions as well as applications to other areas such as Logic, Computer Science and Medicine.

Since their formation as branches of mathematics, Group Theory and Topology intertwine and go hand in hand: one way of understanding the structure of topological spaces is via their group of symmetries, and a fruitful way of understanding the algebraic structure of a group is by making it act on a topological space that one understands. This duality was key in many exponents of modern mathematics; it suffices to mention the recent solution of the virtually fibred conjecture by Ian Agol, who was awarded the 2016 Breakthrough Prize “For spectacular contributions to low-dimensional topology and geometric group theory”.

This new paradigm is clearly reflected in the consolidated research group “Groups, Topology and Applications” of the University of the Basque Country. Research lines of our group cover pointfree and fuzzy topology, finite and profinite groups, combinatorial and geometric group theory, groups of automorphisms of various geometric and algebraic objects, applications of group theory to problems in low-dimensional topology, theory of manifolds, universal algebra and logic as well as representation theory, algebraic combinatorics and design of vaccines.

GRECA: Groups, Representations and Algebraic Combinatorics

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KEY WORDS: Finite p-groups, pro-p groups, characters, representations, algebraic combinatorics.

The research of this group is organised around four main areas, which we describe below:

1. Finite p-groups and pro-p groups

In the case of finite p-groups, we focus on the following two topics: the power structure, and the conjugacy classes, both of elements and subgroups. On the other hand, pro-p groups is one of the most trendy research topics in group theory. These groups provide a way of studying simultaneously a family of finite p-groups whose order grows to infinity. In this field, we are working on several problems: power structure, (co)homology, and word problems such as the width of a word and the effect of a positive law on the values of a word

2. Geometric group theory and first order theory of groups

This is a new area in the research interests of the group, opened up after the arrival to the group of the ERC Starting Grant holder Ilya Kazachkov. In this case we are particularly interested on partially commutative groups, a class of groups defined via commutation relations given by a graph, that generalises both free abelian groups and free groups, and also on limit groups over partially commutative groups. Our goal is to study these families of groups both from an algebraic and an algorithmic point of view.

3. Characters

We work on several problems related to characters and representations, mainly on finite p-groups. Even if the representations of classical groups over finite fields are well understood, there is not a satisfactory theory of the representations of their Sylow p-subgroups, and we are interested in this problem. In another direction, we are analysing how the degrees of the irreducible representations or the values taken by the characters have an influence on the structure of a finite group.

4. Algebraic Combinatorics

We look for t-designs, and more specifically 2-designs, that have nice symmetry properties, in the sense that they admit a group of automorphisms that acts regularly on its points. We are also working on the construction of combinatorial structures linked to differences in finite groups, such as difference sets, difference families, and cyclic association schemes.

QUÍMICA



Electronic spectroscopy, fluorescence microscopy and atomistic simulation of multifunctional dyes and materials

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KEY WORDS: Spectroscopy, Fluorescence Microscopy, Laser Dyes, Zeolite L, AlPOs, MOFs, Clays, Atomistic Simulation, Photosensitizers, Nanoparticles, Photodynamic Therapy, Chirality, Fluorescence Sensors, Antenna materials, White-Light

The research scope of the Molecular Spectroscopy Group is focused on the structural and photophysical characterization of dyes in solution or occluded into nanostructured solid materials (porous like zeolite, aluminophosphates, AlPO, and metal-organic frameworks, MOF, or layered such as clays), as well as grafted to nanoparticles, towards optoelectronic and biophotonic applications. To this aim our laboratory is equipped with advanced and sophisticated light absorption and fluorescence spectrophotometers, confocal fluorescent microscope and flash-photolysis. The experimental characterization is simultaneously complemented with theoretical simulations of the aforementioned dyes and materials to unravel their spectroscopic signatures and to help in the development of novel tailor-made materials.

Our research activity can be summarized in three main blocks as follows:

1. **UV-Vis-NIR Spectroscopy of Organic Dyes.** A rational design of the molecular structure allows the development of multifunctional fluorophores, valid for a wide range of technological purposes. In this regard, the dyes known as BODIPY stand out by their chemical versatility. Thus, taking the boron-dipyrro core as scaffold a wide library of luminophores can be attained, in which the functionalization pattern rules the final photophysical properties of the chromophore. The spectroscopic characterization of these novel BODIPYs decodes the underlying mechanism which explains their behavior as tunable laser dyes, fluorescence molecular probes and sensors for bioimaging, light harvesting assemblies for molecular antennas, optically active molecules in chiroptics and singlet oxygen photosensitizers for photodynamic therapy.
2. **Photoactive Hybrid Materials and Confocal Fluorescence Microscopy.** Some of the above developed organic dyes are occluded into (zeolitic materials, clays, MOFs or silica monoliths) or linked to (silica nanoparticles) solid hosts to yield photoactive hybrid materials with improved photostability, organization and alignment. Moreover, the careful choice of the guest-host pair modulates the fluorescence response of the customized material. Our efforts, which sometimes include the synthesis of the host inorganic framework (zeolites and silica nanoparticles) are focused on the development of solid materials as active media of tunable dye lasers, white-light emitting devices, antenna systems, non-linear optics and for biomedical purposes.
3. **Atomistic Simulation.** The experimental studies are supplemented with theoretical calculation of simple molecules, solutions or solids at different calculation levels; from sophisticated and accurate ab-initio and post-Hartree-Fock methods, based on quantum mechanics, to molecular dynamics or Monte Carlo methods, based on classic mechanics, which allow handling a large amount of atoms. Theoretical simulations provide key information about the structural and electronic properties of the aforementioned organic dyes and hybrid materials, as well as to plan the next generation of photoactive systems.

Rediscovering new porous materials

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KEY WORDS: SMOF, nucleobases, porosity, adsorption, magnetism.

The present work provides a novel synthesis approach to obtain a new type of porous material based on supramolecular interactions called SMOF (supramolecular metal-organic frameworks). These compounds are related to the well-known MOF (metal-organic frameworks) but instead of being sustained by coordinate bonds, the metal-organic structural units are linked by hydrogen bond pairing interactions and/or π - π interactions in such a way that the growth of 3D supramolecular network renders an open-structure. Our research work has enabled us to establish the principles to successfully design and synthesise SMOFs, which are summarised in the following key factors:

1. The use of rigid metal-organic entities as building units, in which the rigidity is accomplished by at least the establishment of two coordination bonds or one coordination bond and a hydrogen-bond intramolecular bond.
2. The establishment of predictable and rigid synthons between the building units like double or triple complementary hydrogen bonding interactions.
3. The non-coplanarity of functional groups involved in the predictable synthons with the purpose of obtaining three-dimensional extended porous supramolecular assemblies.

In order to fulfil the above mentioned prerequisites, we have selected metal-nucleobase entities as building units due to the ability of these N-ligands to establish multiple coordination bonds with metal ions and base pairing interactions. The suitability of this synthetic strategy supported by several SMOFs, in which the structure design factors and synthesis conditions are considered.

Moreover, the SMOFs are exhaustively characterized by thermal analysis, adsorption and magnetic measurements. Thermal analysis reveals that the stability of SMOFs is similar to the conventional MOFs. Regarding the adsorption properties all the present materials are microporous with computed specific surface areas 800 - 3600 m²/g. It must be pointed out, that some of the studied examples are highly selective toward carbon dioxide adsorption when compared to dinitrogen, methane or hydrogen adsorption.

Finally, among the herein presented SMOFs, there is one consisting of heptanuclear Cu(II) wheel entities which have interesting magnetic properties. The inspection magnetic susceptibility curves indicates that the central copper(II) center is antiferromagnetically coupled to external copper(II) centers which are ferromagnetically coupled among them leading to a $S = 5/2$ ground state.

FARMARTEM: Development of new analytical methodologies applied to drug analysis, Metabolomics, environmental, industrial analysis and forensics

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KEY WORDS: drug analysis, metabolomics, pesticides, microencapsulation, fluorinated compounds, documents

FARMARTEM is an analytical chemistry research group involved in the development of analytical methods for different application fields: determination of drugs and metabolomic studies, environmental and industrial analysis, and forensic studies of documents.

Different analytical instrumental techniques are used in the different research lines of this group. Among the separation techniques, ion chromatography has been applied to the determination of anionic inorganic impurities in tough matrixes as the fluorinated inorganic compounds; moreover several inorganic anions and herbicides as glyphosate have been analyzed in underground and superficial water. In the field of drug analysis, capillary zone electrophoresis has been used for the determination of abuse drugs (amphetamines) in hair and liquid chromatography coupled to different kind of detections: photodiode-array, fluorescence and mass spectrometry has been the chosen technique for the development and validation of analytical methods for the detection and quantification of drugs (fentanyl, dobutamine, cardiovascular drugs, ...) in biological fluids (plasma, urine, cerebrospinal fluid, dried blood spots). These methods have been applied to pharmacokinetic, toxicological and monitorization studies. Several sample treatments have been optimized for biological matrixes analysis as solid-phase extraction (SPE), extraction from dried blood spots (DBS), liquid-liquid extraction, solid phase microextraction (SPME) and protein precipitation.

Metabolomics is one of the emergent research lines of the group and targeted and untargeted metabolomics studies have been carried. In this sense, the analytical platform liquid chromatography-mass spectrometry has been used in this research line. Targeted studies of endogenous metabolites (carbohydrates, steroids) in plasma and untargeted ones of metabolic profiles in several fluids (plasma, urine) have been done with the aim of searching biomarkers of disease as schizophrenia or to study the metabolic differences related with the maturation processes in pediatric population.

Gas-chromatography-mass spectrometry (GC/MS) has been the analytical technique utilized for a comparative study of volatiles compounds profiles of intact and mechanically damaged walnuts with the aim of identifying the possible candidate compounds to be used as attractants of the codling moth (*Cydia pomonella*). The use of this chromatographic technique with head-space loop has allowed validating a method for the study of the controlled release of volatile compounds. Multiple solid-phase microextraction (MHS-SPME) coupled to GC/MS has been employed for the development of the DATINK method for documents dating.

Finally, microencapsulation of biocides and drugs is other research topic of the group. A release and permeability study of drugs used for the glaucoma treatment as timolol is being carried out. An inclusion complex of timolol with cyclodextrins has been synthesized and its controlled release is being studied using dialysis membranes and uv-vis spectrophotometry for the monitorization of the drug.

Organometallics in Synthesis

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KEY WORDS: asymmetric synthesis, organometallics, chemoinformatics

Our group works on Organic Synthesis, mainly in asymmetric synthesis and organometallic chemistry. Our projects are focused on the development of new synthetic methods of heterocyclic systems based mainly on lithium and palladium chemistry for the stereocontrolled formation of carbon-carbon bonds. The group has a solid background in Organic Synthesis, which allows us to face the preparation and structural determination of any kind of organic molecules. Our research interests are summarized in the following lines:

Line 1. Metalation-cyclization sequence in the stereocontrolled synthesis of nitrogen heterocycles

The Parham-type intramolecular reactions for the construction of fused indolizidine and quinolizidine, and tetrahydroquinolines is explored, in order to determine the limitations and scope of the method. The synthetic utility of the procedure has been shown by application to the synthesis of a variety of products with relevant biological activities, natural products or analogues.

Line 2. Palladium-catalyzed reactions in the synthesis of heterocycles

The application of palladium-catalyzed C-C bond forming reactions for the synthesis of heterocyclic systems is also being studied. We have shown that competition between intramolecular Heck and direct arylation reactions can be controlled in polifunctional systems. The procedure can be applied to the synthesis of medium-size rings, such as pyrroloazepine and azocine. Asymmetric variants and cascade reactions have also been developed.

Line 3. Enantioselective alpha-amidoalkylation reactions

The Parham cyclization-enantioselective intermolecular alpha-amidoalkylation and organolithium addition-enantioselective intramolecular alpha-amidoalkylation sequences provide a novel synthesis of enantioenriched substituted fused isoquinoline systems. The enantioselection is controlled by using sterically demanding Brønsted acids transition-metal complexes as catalysts.

Line 4. New computational models for the prediction of chemical reactivity, biological activity and toxicity

We are also developing new computational multi-target QSRR methods capable of predicting enantioselectivity levels of a given reaction when structural modifications (on substrates, ligands or catalysts) or experimental conditions are carried out. On the other hand, multi-target QSAR (quantitative structure-activity relationship) or QSTR (structure-toxicity relationship) models are also be carried out.

For reviews on our work, see: Eur. J. Org. Chem. **2011**, 3610; *Carbolithiation of carbon-carbon multiple bonds, en Science of Synthesis. Knowledge Updates 2011/4*, D. G. Hall, K. Ishihara, J. J. Li, I. Marek, M. North, E. Schaumann, S. M. Weinreb, M. Yus, Eds.; Thieme: Stuttgart, **2012**, p. 191. *Beilstein J. Org. Chem.* **2013**, 9, 313.

For some selected publications: RSC Adv. **2016**, 6, 38602; *Eur. J. Org. Chem.* **2016**, 2054; *Adv. Synth. Catal.* **2015**, 357, 3206; *Adv. Synth. Catal.* **2015**, 357, 463; *Adv. Synth. Catal.* **2014**, 356, 1853; *Curr. Drug Metabolism* **2014**, 15, 470; *Curr. Top. Med. Chem.* **2013**, 13, 619; *Eur. J. Org. Chem.* **2013**, 3013; *Curr. Top. Med. Chem.* **2013**, 13, 1713; *Eur. J. Org. Chem.* **2013**, 1460; *J. Org. Chem.* **2012**, 77, 2986.

More detailed information can be found in our web page: www.ehu.es/oms

Polyoxometalates (POMs). Building Blocks for Advanced Functional Materials

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KEY WORDS: Polyoxometalates, Functional materials, Smart surfaces.

Polyoxometalates (POMs) are a well-known class of metal-oxo anionic clusters that encompasses species with a large variety of shapes and compositions, as well as applications in fields of current technological, economic, and environmental interest (e.g., catalysis, medicine, energy, materials science). The use of POM frameworks as multidentate O-donor ligands to incorporate either functional organic moieties or additional 3d- or 4f-metal centers in the inorganic skeleton represents a powerful tool to design new architectures with remarkable properties. Owing to their interesting features (high solution and thermal stability, high acidity, versatile redox properties), POMs are ideal candidates to be incorporated as active groups in the formation of advanced functional materials.

As much as four different research lines mainly focused on the synthesis and structural characterization of POM-based materials are currently being developed in our group:

3d/4f METAL CONTAINING POM ASSEMBLIES

Metal-containing species constitute one of the largest and currently most active groups within the POM chemistry because combination of POM building blocks with 3d- and/or 4f-metals has been shown to be a powerful tool for designing new architectures and introducing additional functionalities to the system. Our newly synthesized polyanions have shown interesting photoluminescent- and catalytic properties for the heterogeneous selective oxidation of aniline, as well as the ability to self-assemble in diluted aqueous solutions into hollow, spherical and single-layered blackberry-type structures.

ORGANIC DERIVATIZATION OF POMs

The organic derivatization of POMs has been identified as a key factor for the clusters to be suitably incorporated into functional materials. Different synthetic routes have been explored to prepare solution stable hybrid clusters. These include the use of organo p-block derivatives (organosilyl, -phosphoryl or -stannyl moieties) in combination with lacunary polyoxotungstates and the reactions of POMs with exposed 3d- or 4f-metal centers displaying at least two available coordination sites toward organic ligands with chelating ability. The synergy between both organic and inorganic components has resulted in photoactive materials or single-ion magnets among others.

MULTIFUNCTIONAL HYBRID POMs WITH OPEN FRAMEWORKS

The grafting of discrete coordination complexes with peripheral organic ligands to POM surfaces can result in three-dimensional crystalline frameworks with permanent porosity. The use of first-row transition metal complexes of macrocyclic polyamines in combination with POM clusters usually leads to open hybrid frameworks with interesting functionalities such as selective adsorption of gases and remarkable activity as heterogeneous catalyst. This family of compounds have also shown the ability to respond to external stimuli, in such a way that they can undergo thermally triggered single-crystal-to-single-crystal structural transformations promoted by reversible dehydration processes.

SMART SURFACES

The final goal of this research will be the design of novel polymer/polyoxometalate smart hybrid coatings with a broad scope of potential applications. These hybrid composites are intended to be prepared from the immobilization of POM clusters as the functional active entities on tailored polymeric films with reactive groups at the interface via classical coordination chemistry. For this purpose, we have selected polystyrene surfaces with terminal polyacrylic functionalities and POMs with exposed 3d/4f metal centers. Their preparation will be mainly focused in the search of catalytic, magnetic or luminescent properties depending on the functionality of the immobilized POM species.

Polymers: answers for XXI. Advanced Manufacturing and waste treatment

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KEY WORDS: Polymers, Advanced manufacturing, 3D-printing, shape memory, nanoparticles, ground remediation.

The European Union estimated that manufacturing represents 20% of the EU's employments, that is, over 30 million of EU's citizens work in industry. Also, it is to be notice that each of these industrial jobs is connected to, at least, two service related jobs. However, in the last years the leadership of the European manufacturing has been threat by several emerging or renovated potencies. The battle with the lower-wage economies is already loss, so the main effort of the EU it is focused on the creation of high added value in order to relaunch the European manufacturing and economy.

Between the research lines of Macromolecular Chemistry Group of the department of Physical Chemistry of the Faculty of Science and Technology (UPV/EHU), two of them are focus in Advance manufacturing and materials and Waste reduction.

ADVANCE MANUFACTURING AND MATERIALS

1. **3D-PRINTING.** In recent years, 3D printing has been emerging as a promising fabrication technique for many industrial sectors. The versatility this technique, being capable of rapid and on-demand fabrication of sophisticated objects, has focused the interest of some of the most important industrial sectors as automotive or machinery. The 3D-printing could fulfill the lack of additive manufacturing techniques with high resolution and scalable at the same time but also cost effective and rapid.
2. **SHAPE MEMORY POLYMERS.** Shape memory polymers are materials that have the capability to be deformed from permanent shape to a temporally shape. That is, they have the ability to memorize a macroscopic shape. These materials have great potential for application in sensors, actuators or smart devices. Besides, the mechanical properties of the shape memory polymers could enable the development of novel types of medical devices.

WASTE TREATMENT

IRON ZERO VALENT NANOPARTICLES After a major change in Basque Country's industrial network in which some industries had closed down or relocated. Several environmental problems arise, due to the highly contaminated grounds that they leave behinds. One of these pollutant is the Lindane which could induce a serious health problems. In order to clean Lindane contamaminated grounds zero valent iron nanoparticles have been successfully used as an environmental remediation material, capable to eliminate Lindane and its derivates from the ground.

New synthetic methodologies based on sustainable procedures

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KEY WORDS: sustainable chemistry, metal catalysts, hypervalent iodine

The main research lines that are being conducted by our group are focused on the development of new synthetic methodologies to be carried out under sustainable conditions ("green chemistry").

• NEW CATALYSTS FOR MORE EFFICIENT, COST-EFFECTIVE PROCESSES

We design and synthesize new catalysts -mainly based on palladium, copper, nickel or iron- to be used in tiny amounts under sustainable conditions (aqueous or biodegradable media, possible reuse of the catalyst...). Our research has provided excellent results for a variety of transformations as shown in Figure 1. The described optimized methodology has allowed us to prepare a number of polycyclic compounds of interest (see Figure 2) with the benefits of short synthetic sequences, economical advantages, and sustainability when compared to previously reported alternatives.

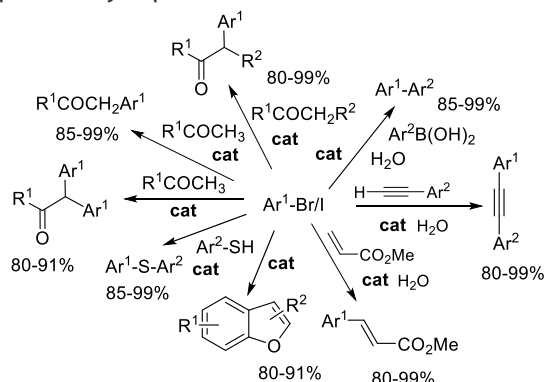


Figure 1. Selected reactions performed in the presence of our new catalysts

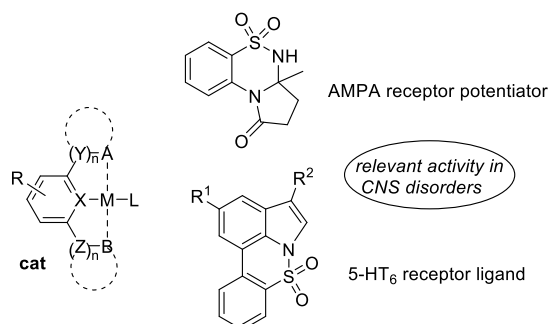
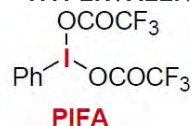


Figure 2. Molecular structure of some of the catalysts employed and relevant synthesized products exhibiting biological activity

• HYPERVALENT IODINE REAGENTS AND MICROWAVE ACCELERATED ORGANIC SYNTHESIS



PIFA, [bis(trifluoroacetoxy)iodobenzene], is an efficient reagent with low toxicity that requires soft reaction conditions. It can be used as a greener alternative to metal catalysts in different processes (see Figure 3). In addition we have introduced the use of microwave reactors in our synthetic plans, with and without the use of I(III) reagents (see Figure 4).

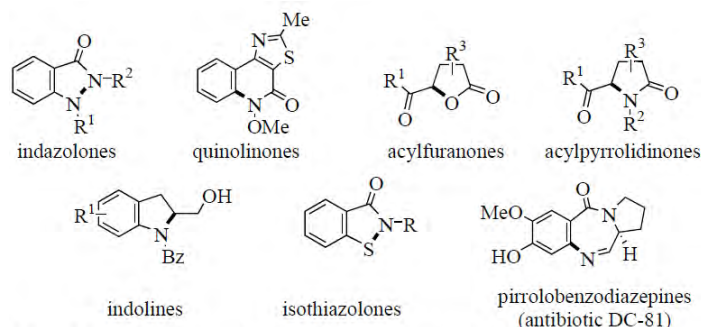


Figure 3. Selected examples of the use of PIFA in heterocyclic synthesis. The bond created by this reagent is highlighted.

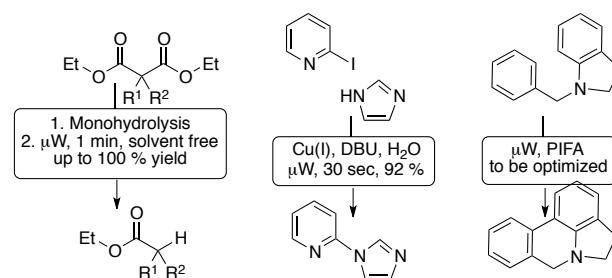


Figure 4: (a) decarboxylation of substituted malonate derivatives; (b) Bis-heteroaryl coupling; (c) heterocyclic synthesis.

Quantum Technologies for Information Science (QUTIS)

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KEY WORDS: quantum physics, quantum optics, quantum information, superconducting circuits, quantum biomimetics, quantum neuromimetics, quantum technologies.

The research group “Quantum Technologies for Information Science (QUTIS)”, led by Prof. Enrique Solano, develops cutting-edge theoretical research for the sake of fundamentals and their implementation in interdisciplinary quantum technologies. We relate concepts in quantum optics, quantum information, superconducting circuits, and quantum biomimetics, among others. QUTIS is a dynamic, hard-working, and creative group with wide interests in arts, physics, and science. We are strongly driven by intellectual curiosity, keeping as our main goal our aesthetic and scientific expression in a friendly competitive environment. At the same time, we constantly search that our original cross-disciplinary ideas have a realistic approach towards experimental implementations. QUTIS is committed to the team-oriented production of novel influential ideas at the international level, where creative ideas merge with quantum technologies.

1. **Quantum information science** is a field that studies the features of quantum effects, and develops techniques to exploit them to outperform classical protocols and devices. In particular, we are interested in combining lines and tools such as entanglement classification, tensor networks, matrix product states, quantum algorithms, algebraic geometry, adiabatic elimination, embedding methods, among others.
2. In 2008, the emergence of the first experimental realization of a memristor, a resistor with memory whose resistance depends on the history of charges crossing the device, meant a technological revolution that promises to radically transform our computational framework. In this context, we wondered how to properly quantize this device in such a way that it is able to deal with quantum information. We are also interested in the possible applications of these quantum memristors not only to quantum computing, what we call **neuromorphic quantum computing**, but also to quantum simulations of non-Markovian, fluid dynamics and, especially, to the implementation of **quantum machine learning** protocols. Indeed, a device with memory seems a natural platform to implement quantum machine learning protocols. We are currently working on implementing quantum memristors in different quantum platforms, quantifying their memory in the framework of non-Markovian processes, and studying how to engineer this memory for implementing quantum machine learning algorithms.
3. **Superconducting qubits** are considered as artificial atoms made out of superconducting linear and nonlinear devices, and having as their main purpose the build-up of quantum computers and quantum information protocols with quantum circuits. **Circuit quantum electrodynamics** represents the arrival of quantum optics to the microwave domain, via the implementation of coplanar waveguide cavities and transmission lines working at the quantum level due to the use of low cryogenic temperatures. The combination of superconducting qubits and circuit QED has produced the more general field of superconducting circuits, yielding an incredible boost in the development of quantum technologies with microwaves and superconducting mesoscopic systems.
4. **Quantum biomimetics** consists in the design of quantum protocols that recreate in quantum platforms behaviors and properties which correspond to macroscopic biological phenomena. These bio-inspired features, such as self-replication or brain-like memory, are naturally emerging from complex interactions between multiple subsystems, and are not usually described from first principles in physics. Therefore, we reduce them to simple mathematical models and reproduce them at the microscopic quantum scale. Furthermore, we aspire not only to describe these phenomena, but also to make use of them to engineer novel quantum protocols and devices.

The challenge of Mars exploration through Analytical Chemistry

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KEY WORDS: Marte, Raman, Exomars2018, Mars2020, ESA, NASA.

Since 2013, IBeA research group works, through an invitation from the Astrobiology Unit from Valladolid University, in EXOMARS 2018 and MARS 2020 projects on the Mars surface exploration.

In EXOMARS 2018 project, IBeA is part of the Science group which, among others, has as objective the study of terrestrial analogues of Mars surface geology using different meteorites landed in the Earth and coming from the Mars crust. Moreover, in a near future, data sent to the Earth by the rover from the Red Planet will be also interpreted by the research group. In these studies, Raman spectroscopy will be a very useful tool. Actually, a Raman spectrometer will be sent for the very first time inside the EXOMARS 2018 rover for the study of the Mars geology, and the possible biology, present on its surface. This Raman device has been developed by the Astrobiology group from Valladolid University.

Up to now, several terrestrial analogues and meteorites have been studied by IBeA. Some of those analyzed meteorites are nowadays in possession of the research group thanks to the agreement (2014) between NASA and UPV/EHU. The others were acquired by IBeA research group inside CamOnMars project and they are already part of the UPV/EHU collection.

One of the challenges that must be tackled in this project will be to know if the studies performed on Earth using the Raman spectrometer developed by Valladolid University have or will have validity on Mars, since the pressure, temperature and the different composition of the atmosphere could vary the response of the equipment. Another challenge of the mission will be to search for life or signs of past life through the analytic signals of the biomolecules.

In MARS 2020, IBeA is part of the group working on the development of calibration target for the SuperCAM instrument that is one of the nine instruments present in the rover. The SuperCAM device includes: Laser Induced Breakdown Spectroscopy (LIBS), Raman Spectroscopy, Time-Resolved Fluorescence, Infrared and Visible Reflectance spectroscopy and a high-resolution camera. The perfect calibration of the different instruments is essential for the scientific success of the mission. The calibration target bracket will be manufactured in Euskadi (AVS Enterprise, Elgoibar) with whom IBeA collaborates since 2014.

Several challenges must be fulfilled in the preparation of the calibration target. On the one hand, a selection of the most suitable materials for the calibration of all instruments must be performed. Besides, the mechanic resistance of those materials must be checked. The materials will pass a very exigent mechanic tests which will pretend launching, flying and landing conditions of the rover. Moreover, selected samples must resist Mars conditions.

On the other hand, once the compounds are approved, they must be prepared fulfilling very demanding homogeneity tests that will validate them as reference materials for the calibration process. This task will be performed by IBeA research group by using Raman and EDXRF image techniques.

Nanostructured Materials for Energy and Biomedical Applications

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KEY WORDS: Li-ion and Na ion batteries, electrochemistry, spinel, sodium vanadium fluorophosphates, nanoparticles, thermal decomposition, superparamagnetism, electron magnetic resonance, magnetic hyperthermia

The work developed in this research group can be divided in two main lines: functionalized magnetic nanoparticles for biomedical applications and materials for energy. The first one explores magnetic nanoparticles for their application in the research field of biomedicine. The size confinement to nanometer scale in magnetic materials changes the properties from those of the bulk ferro and ferrimagnetic counterparts. These properties are interesting for some biomedical applications, such as drug delivery, MRI contrast or magnetic hyperthermia. In magnetic hyperthermia, an emerging alternative for the treatment of cancer, the size of nanoparticles, their stabilization and biocompatibility are key attributes that must be controlled. In this sense, nanoparticles must be in a biological environment, requiring a proper optimization of the synthesis method and an adequate surface functionalization, which allows a good stability.

The most usual materials for such applications are the superparamagnetic iron oxide (SPIO) compounds, which have inverse spinel structure. Specifically, our work is focused on Fe₃O₄ nanoparticles and nickel or manganese ferrites with different compositions to study the changes in magnetic properties. The proper functionalization of these nanostructures with polymer ligands as PMAO or kitosane render hydrosoluble particles which are additionally functionalized with biomolecules to enhance targeting or delivering.

The second aspect covered by the group is the search for commercially viable Li-ion and Na-ion batteries, that is, more economic, safer and longer-life batteries. A substantial segment of the battery materials community is moving toward developing electrode materials on the basis of abundance and availability of the relevant chemicals. Regarding to lithium ion batteries, lithium manganese oxide spinel is especially interesting for use in hybrid electric vehicles and electric vehicles due to its low cost and high safety. However, the main problem for application is the capacity fading caused by the instability of Mn(III). In order to improve that factor, we investigate the effect of substitution of a small quantity of Mn by p-block elements such as Ga³⁺ or Si⁴⁺, Li(Mn,M)₂O₄ (M = Ga³⁺, Si⁴⁺).

On the other hand, the low cost, high abundance and ease of acquisition of sodium minerals promote interest in sodium-based electrochemical systems, especially for stationary energy storage devices. However, significant challenges such as energy density and long term stability must be addressed. Na₃V₂O_{2x}(PO₄)₂F_{3-2x} sodium-vanadium fluorophosphates are good cathodic materials for Na-ion batteries due to their high reaction voltages (at 3.6 and 4.1 V vs. Na/Na⁺) and their good specific capacity values in sodium half-cells (theoretical specific capacity of about 130 mAh/g) which leads to high energy density compounds (ca. 500 Wh/kg). Metal-air batteries are also studied due to their high energy density compared to traditional energy storage systems.

Characterization of the different materials comprises powder X-ray diffraction (XRD), thermogravimetric analysis, Dynamic Light Scattering (DLS), Scanning and Transmission Electron Microscopy (SEM/TEM) and magnetic susceptibility measurements and Electron Magnetic Resonance Spectroscopy (EMR). Hyperthermia measurements are performed for nanoparticles with the highest magnetization values. The electrochemical measurements are conducted using coin-cell and Swagelok-type cells *versus* a metallic lithium or sodium anode.

Configuration interaction wave functions: Excitation based and seniority number based approaches

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KEY WORDS: Configuration Interaction. Seniority number. Convergence of wavefunctions.

SUMMARY

It is well known that the wave functions of N-electron systems arising from the full configuration interaction (FCI) treatment are the exact solutions of the Schrödinger equation for a given basis set. However, their determination requires a computational effort too high in most practical situations. To reduce this cost one formulates expansions of configuration interaction (CI) in which only a limited number of N-electron Slater determinants is taken into account. The most popular criterion to select these determinants is based on the particle-hole excitation level from a reference determinant, although other procedures, as the seniority number of the determinants, have also been used. We have studied the configuration interaction (CI) method when an N-electron Hamiltonian is projected on Slater determinants selected according to their seniority number value (Ω)^{1,2}. The formulation of the seniority number and the N-electron spin-squared operators in terms of spin-free replacement operators³ allows us to analyze the spin features of the wave functions provided by that procedure, showing that they have no spin contamination³. The computational cost is evaluated in terms of the size of the matrices required to implement this treatment in any system, for any spin symmetry. The performance of these seniority-number-based CI expansions in several molecular orbital bases is also investigated^{4,5}. Our results indicate that the basis set in which the seniority number operator expectation value is minimum (M_{\min}) leads to energy values closer to those provided by the FCI level. A hybrid CI treatment ($CI_{\Omega=0,SD}$) based on both seniority number and excitation schemes has also been investigated⁴, showing its adequacy to describe systems which exhibit dynamic correlation at determined geometrical arrangements but show static correlation at other arrangements.

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Natural products in agricultural foods, beverages and plants

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KEY WORDS: Polyphenols, anthocyanins, red wine, fruits, vegetables, beverages, cider, honey, olive oil, agricultural food products, agricultural by-products, nutraceuticals, antioxidant, antimicrobial activity, antiparasitic activity, encapsulation

Determination of the chemical composition of foods and beverages has a huge interest from many points of view. A deep knowledge of natural products in foods can lead to improve nutritional quality, manufacturing methods, or to detect geographical origins, bad practices, adulterations and frauds.

Polyphenols are a very important group of natural products due to their ubiquity in the Plant Kingdom, and their interest as a key to explain many food properties such as flavor, bitterness, astringency, aroma and color, besides their known beneficial effects on human health (e.g. lower risk of heart diseases and cancer).

In this regard, and after successful works in beverages such as ciders and wines, apples, fruit juices, edible oils, coffee, microalga, cianobacteria and medicinal plants, our research group is currently working in the following projects:

- Anthocyanin and tannins analysis in red wines and in extracts of freeze-dried grape pomace in order to (i) evaluate and control vinification procedures; (ii) study the influence of microoxygenation and ionic exchange techniques on the vinification procedure; (iii) evaluate the influence of enological factors and climatology on different grape varieties and monovarietal wines; and (iv) be used as quality parameters related to local Protected Designation of Origin, such as wine color, which is one of the most important parameters directly related to anthocyanins.
- Volatile compounds analysis in red wines by *fast* gas chromatography: Volatiles are responsible for wine aroma, which is a feature that provides information to the wineries about the course of vinification, a critical process for the final quality of wine. The effect of enological techniques such as microoxygenation and ionic exchange, as well as the use of minor native grape varieties on wine aroma are being studied in order to evaluate the influence of climate change on wine quality.
- Characterization of the polyphenolic profiles of agricultural food products determined by HPLC-DAD and UHPLC-DAD-QTOF/MS: Polyphenolic composition together with chemometrics (PCA, LDA, PLS-DA, PLS, neural networks) provides useful tools for quality control, authentication and detection of adulterations of agricultural food products (fruits, vegetables, fruit derived foods, cider, wine, honey, olive oil); detection of bad practices in food manufacturing (olive oil); optimization of production technologies to obtain foods (lettuce) with high phytochemical quality; and development of novel rapid methods to determine polyphenol composition of agricultural foods (wine, honey) by vibrational spectroscopies and regression models.
- Multivariate data analysis of the polyphenolic profiles of apples, together with QTLs and molecular markers for the selection of genotypes with high fruit (apples) quality and interesting agro-technological properties such as resistance to biotic agents and regular productivity; with genome-wide association (GWAS) for the detection of important SNPs in the formation of phenolic compounds belonging to the leading polyphenol families as a tool for the selection of new varieties with specific phenolic composition in the process of genomic selection in new generation of crossovers improvement; and for the technological characterization of apple varieties.
- Valorization of agricultural food by-products (apple pomace, grape pomace, olive pomace) generated during manufacturing processes by food industry to obtain high value-added bioactive molecules for the food, pharmaceutical and cosmetic industries, as well as for veterinary use, for instance in bee health to control, prevent and fight bee diseases such as American foulbrood or varroasis.
- Encapsulation of polyphenols and polyphenolic extracts of agricultural food by-products for different applications, food additives, veterinary use, nutraceuticals, etc.
- Natural products in plants, microalgae and cianobacteria in the search of high value-added bioactive compounds for the food, pharmaceutical and/or cosmetic industries.

Group of Asymmetric Synthesis, Sustainable Chemistry and Biomimetic Processes

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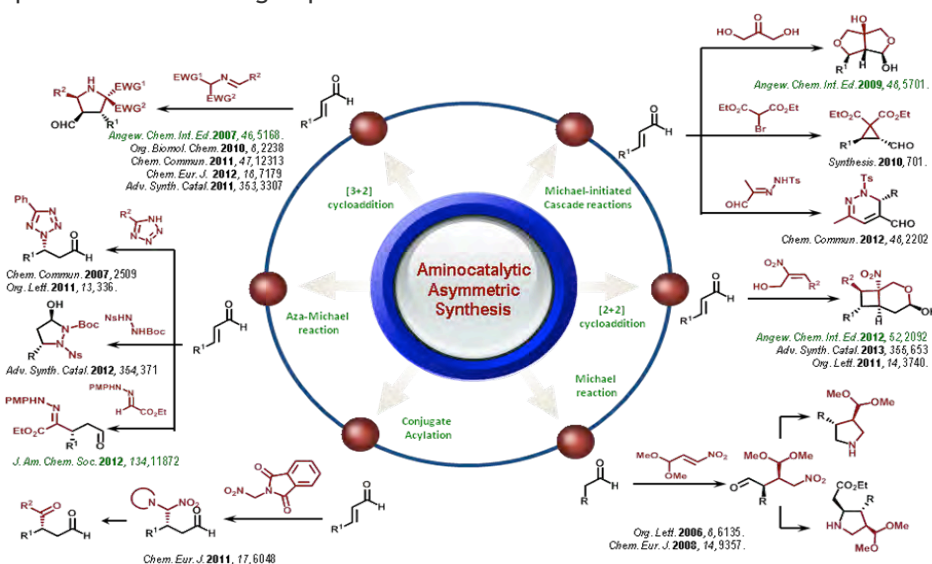
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KEY WORDS: Organocatalysis, Sustainable Chemistry, Green Chemistry, Chiral Drug Synthesis, Biomimetic Processes.

Observing how Mother Nature solves complex problems in an easy way, the human being has been trying to imitate it for many centuries. Thus, the high catalytic efficiency of several enzymes in many natural processes has inspired many researchers to imitate and even improve its action, creating new protein-based biocatalysts. However, these show a rather narrow scope due to the inherent specificity of the biologic processes. For this reason, new and more flexible catalytic systems are needed for fine chemical production.

In asymmetric synthesis, not only should the catalyst accelerate the reaction but it also should be very stereoselective and flexible, in order to allow its use for the synthesis of different target molecules. In the last decade, organocatalysis has emerged as a very efficient tool in organic synthesis using small chiral organic molecules, which activate both reagents and reactants responsible for the stereocontrol of the reaction, in the absence of any metal. These organocatalysts are stable in air, water-compatible and easily prepared in both enantiomeric forms. Furthermore, most of them are commercially available, showing a great advantage when employed by pharma- and agrochemical industry, due to the fact that the presence of traces of contaminating transition metals is absolutely forbidden by legal regulations, avoiding additional purification methods.

Our research in this field has prompted us to study several organocatalytic methodologies and to the design of new catalysts which allow to carry out the reaction in water. These findings, together with the previously described advantages of organocatalysis compared to traditional metal catalytic reactions, are in accordance with the principles of Green Chemistry. Some of the following examples show the utility and the synthetic applications developed in our research group.



Our experience in Asymmetric Synthesis is well known and internationally recognized. Our research group provides laboratory facilities for students in the last year of degree, Master students, PhD. students or post-doctoral researchers. More information can be found in the group web page (<http://www.ehu.es/GSA>).

Environmental metabolomics: A new challenge in analytical chemistry

Ekhiñe Bizkarguenaga¹, Laura Blanco-Zubiagirre¹, Alberto de Diego^{1,2}, Nestor Etxebarria^{1,2}, Luis Angel Fernández^{1,2}, Mireia Irazola¹, Leire Mijangos¹, Maitane Olivares^{1,2}, Ailette Prieto^{1,2}, Oihana Ros¹, Aresatz Usobiaga^{1,2}, Itsaso Zabaleta¹, Haizea Ziarrusta¹, Olatz Zuloaga^{1,2}

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² Research Centre for Experimental Marine Biology and Biotechnology, PIE-UPV/EHU.

KEY WORDS: environmental metabolomics, non-target analysis, bioinformatics.

We live together with the surrounding chemicals without grasping very well their fate and behaviour in the environment, and essentially their effects on the living organisms. Consequently, we deal with the risks for the environmental and the human health associated to the presence of many contaminants. This kind of issue requires a multidisciplinary and an integrative approach including chemists, biochemists, toxicologists, biologists and physicians, among many others, to provide the understandings of the processes that take part from the release of any contaminant in any media to the effect observed in organisms, communities and ecosystems.

The growing use of the omic sciences in many disciplines is also seen in the environmental issues. In the last decade, we witnessed the application of high throughput analytical instrumentation to support the development of the metabolomics. The underlying rationale is that through the comprehensive analysis of the metabolome we are able to uncover the mechanisms of action of known pollutants, new biomarkers of exposure to chemical or physical stress, or the most likely adverse outcome pathways affected by the exposure to any contaminant.

In this sense, both at the Faculty of Sciences and Technology and Plentzia Marine Station, we are currently working on (i) the development of analytical methods for emerging pollutants through high resolution chromatographic techniques, (ii) the use of passive sampling devices to provide integrative levels of the presence of many contaminants in aquatic and atmospheric media, (iii) on the plant bioavailability processes of some emerging pollutants that can be amended through contaminated sewage sludge that is used as fertilizers and the effect of that bioavailability on human consumption, and finally, (iv) we are also studying the variation of the metabolic profiles in marine organisms when they are exposed to different contaminants.

Regarding the last research line, we make use of the facilities of the PiE to run the controlled exposure experiments and to carry out the dissection of the fishes. Essentially, we collect the muscle, liver, gills, brain among the tissues and the plasma and bile among the biofluids. All the samples are snap frozen in liquid nitrogen as soon as they are obtained and they are stored at -80°C until the analysis. The analytical procedure is carried out following a well-established work-flow assuring the integrity of the samples and analytes. Since the variability of the metabolome is highly dependent on the phenotype of each organism and the surrounding conditions, to attribute any variation of the metabolome to known and controlled experimental variables, the number of samples and individuals needed to carry out this type of studies is very demanding. Finally, each sample can be split into several extracts according to the analytical outcome, i.e. polar and non-polar extracts, to measure target metabolites or to run non-target analysis, or transformation products of the contaminants, or to follow a LC-HRMS, a GC-MS or H-NMR analysis.

Finally, based on the analytical data (quantitative results, spectra, pathways, etc.), a statistical differential analysis is typically carried out to obtain the most likely chemical features of the samples and to link those features with the metabolic pathways. Eventually this process would end up by the identification of the mechanisms of action triggered by the exposition to a known contaminant.

Advanced spectroscopic techniques applied to solving chemical problems

Imanol Usabiaga, Pedro Felipe Arnaiz, Jorge González, Roberto Fernández, Jone Garate, Iciar Uriarte, Montserrat Vallejo, David Olivenza, Marta Fernández, Virginia Ovejas, Raúl Montero, José Andrés Fernández, Asier Longarte, Emilio Cocinero, Francisco J. Basterretxea

KEY WORDS: spectroscopy, chemistry, biochemistry.

A variety of high resolution and time-resolved spectroscopic techniques involving coherent radiation is presented, and their contribution to solving different problems of interest in chemistry and biochemistry is presented. Using electronic laser spectroscopy in supersonic jets, molecular systems of biological interest can be studied, such as stable molecules and intermolecular complexes bonded by non-covalent interactions. Rotational spectroscopy in the microwave region is a very high resolution technique that allows discriminating molecular structures in the gas phase, which are of interest in astrochemistry and biology, such as ribose. Femtosecond time-resolved laser spectroscopy allows to follow the ultrafast dynamics of the excited states of a variety of species, such as aromatic chromophores or prebiotic molecules, either in the gas phase or in solution. Finally, the combination of Fourier-transform infrared spectroscopy and microwave spectroscopy applies to the study of physico-chemical processes in atmospheric science, like hygroscopic and reactive properties of tropospheric aerosols and nucleation processes in secondary aerosols.

INGENIERITZA KIMIKOA

INGENIERÍA QUÍMICA



Natural resources sustainability: Challenges in clean and safe energy

J. I. Álvarez-Uriarte, A. Aranzabal, J. L. Ayastuy, Z. Boukha, J. M. Castresana-Pelayo, A. Choya, U. De La Torre, B. De Rivas, M. Gallastegi-Villa, M. Gil-Calvo, J. A. González-Marcos, M. P. González-Marcos, J. González-Prior, J. R. González Velasco, M. A. Gutiérrez-Ortiz, J. I. Gutiérrez-Ortiz, A. Iglesias, C. Jiménez-González, R. López-Fonseca, A. Morales-Marín, J. A. Onrubia, B. Pereda-Ayo, A. Quindimil, A. Reynoso, A. Salbidegoitia, M. Urrutxua

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KEY WORDS: Hydrogen production, SR, APR, biomass, glycerol, CO-PROX, WGS, OWGS.

The increasing economic development in the world has brought an increase in energy consumption, so it is necessary to develop a new energy map where renewable energies would occupy a prominent place to meet the demand and assure the energy supply, protecting the environment. In addition to reducing air pollution and emissions of greenhouse gases, the use of hydrogen as an “energy vector” would reduce the current dependence on fossil fuels, thus promoting the development of fuel cell technology (particularly in the transport sector).

Hydrogen, as new energy vector, will be the main energy supply by means of the fuel cells in the near future. TQSA research group has focused its efforts on the development of catalysts for producing H₂ –rich streams from different types of gas-phase reforming (POX (Partial Oxidation), SR (Steam Reforming), OSR (Oxidative Steam Reforming)—from hydrocarbons of different nature —natural gas (CH₄), petrol (*i*-C₈H₁₈), diesel (*n*-C₁₄H₃₀)—.

The use of hydrogen, derived from biomass using processes, in the fuel cell technology, allows a net zero emission of CO₂. The production of biodiesel generates an abundant availability of liquid phase glycerol. Aqueous streams in the petrochemical industry also contain a large amount of difficult to separate hydrocarbons. The catalytic reforming of such streams through the proposed technology will allow its valorization through conversion into hydrogen.

Among the catalysts developed for this purpose, NiAl O₄(Al₂O₃), obtained from the nickel aluminate spinel, offers several advantages in reforming processes, such as high catalytic stability and high metal dispersion after reduction at high temperature. These catalysts have been tested in their traditional powder form, but the objective now is to incorporate them in structured metallic wire mesh catalysts, which would allow working at higher space velocity with a minimal pressure drop.

The H₂ produced is then fed to the fuel cell. Since the fuel cell has a low tolerance for CO and its content in the hydrogen stream should be minimized (<1 ppm under stationary conditions and <25 ppm for specific peaks), a prior purification to reduce the content of CO and enrich the H stream is required, first by water gas shift reactions (WGS) and then by CO oxidation (CO-PROX), thus preventing poisoning.

The most viable alternative during the transition to the widespread use of hydrogen in automotive is the on-board production. Therefore, our aim is the *in situ* generation of H₂ and the design of a catalytic converter to perform both the WGS reaction and CO-PROX reaction, i. e. the Oxygen-enhanced WGS (OWGS), in order to purify the hydrogen stream from the hydrocarbon reforming. In this way, the volume of the converter could be reduced, thus making it more viable for its employment in the automotive industry.

Bimetallic Au-Co₃O₄/CeO and Au-CuO/CeO catalysts have been synthesized for this OWGS process, achieving higher conversions than those obtained in the WGS reaction. In order to reduce both the cost and the converter size, the catalysts have been incorporated into monolithic structures, which allow working at higher space velocity, thus getting higher conversions than those obtained with the powder catalysts.

Challenges in actions on climate change and sources and raw materials utilization

J. I. Álvarez-Uriarte, A. Aranzabal, J. L. Ayastuy, Z. Boukha, J. M. Castresana-Pelayo, A. Choya, U. De La Torre, B. De Rivas, M. Gallastegi-Villa, M. Gil-Calvo, J. A. González-Marcos, M. P. González-Marcos, J. González-Prior, J. R. González Velasco, M. A. Gutiérrez-Ortiz, J. I. Gutiérrez-Ortiz, A. Iglesias, C. Jiménez-González, R. López-Fonseca, A. Morales-Marín, J. A. Onrubia, B. Pereda-Ayo, A. Quindimil, A. Reynoso, A. Salbidegoitia, M. Urrutxua
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KEY WORDS: environmental catalysis, NSR, SCR, NO_x removal, CO₂ methanation, P2G

CATALYTIC TECHNOLOGIES FOR POLLUTANTS ABATEMENT FROM STATIONARY AND MOBILE SOURCES

Mobile sources. TQSA does research on two technologies for NO_x removal from diesel engine exhaust gases: NO_x storage and reduction (NSR) and selective catalytic reduction (SCR). The NSR technology requires a catalyst combining NO_x adsorption sites and metallic sites to enhance oxidation and reduction reactions, what is achieved on a Pt-Ba/Al₂O₃ formulation washcoated over cordierite monolith. On the other hand, the SCR technology feeds continuously a reducing agent (NH₃ or hydrocarbon) which is adsorbed on Cu-zeolite catalyst and subsequently reacts with NO_x to selectively form N₂. More recently, we have combined both technologies in two consecutive bed reactors achieving potential zero emission levels of pollutants (CO, HC and NO_x).

Stationary sources. Among the variety of pollutants coming from industrial effluents, we are interested in reduction of methane emissions (energy power plants and natural gas engines), halogenated volatile organic compounds (HVOC in PVC chemical plants, and textile, electronic and metallurgical industries) and dioxins/furanes with NO_x (solid wastes incineration plants). Under this frame, TQSA develops:

1. Catalysts for individual pollutant removal, such as chlorinated volatile organic compounds, or methane from its own combustion in small engines.
2. Catalysts for simultaneous elimination of dioxins (PCCD)/furanes(F) together with NO_x from municipal waste incineration plants.

POWER-TO-GAS: METHANATION OF CO₂ TO PRODUCE SYNTHETIC NATURAL GAS (SNG)

The concept power-to-gas or abbreviated as P2G, is based on the process which is able to produce hydrogen from exceeding electric energy, which is directly introduced into the transport and distribution gas network to be used when demand exists or well is utilized for production of SNG, which is also injected into the mentioned network. Wind, solar or any other renewable energy can be used in the P2G process.

We, at TQSA, are designing catalysts (Ni, Ru) to carry out efficiently the methanation reaction, as well as reactors integrated with heat exchange to allow the capture and valorization of CO₂ generated in industry, by its transformation with renewable H₂ (wind, solar, ...) into SGN that can be used again as fuel in the process boilers, e.g. paper manufacturing industries.

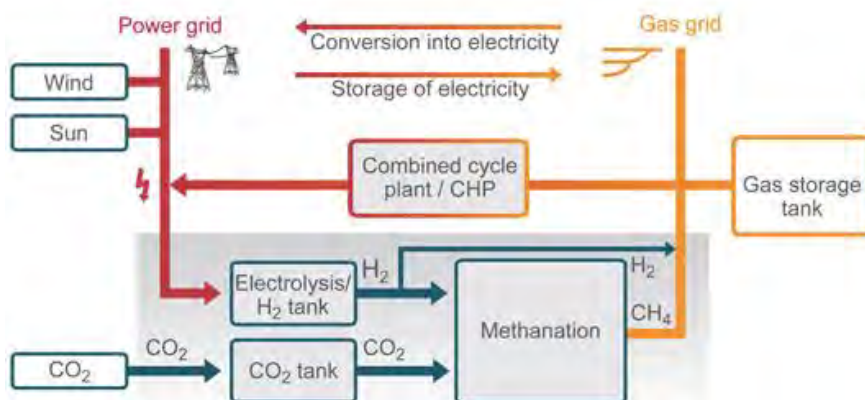


Fig. 1. Schematics of the P2G process.

Reactor and processes for waste valorization

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KEY WORDS: Waste-refinery, spouted bed, reactor

INTRODUCTION AND OBJECTIVES

This research topic of the Catalytic Processes and Waste Valorization (CPWV) research group is focused on the development of new reactors and equipment for the valorization of solid materials that are difficult to handle and wastes (biomass and consumer society wastes), with the aim of adapting their properties (with treatments such as drying) or for obtaining fuels or raw materials, by means of thermal treatments (pyrolysis, gasification), catalytic processes or their combination. These are original processes (lead to patents) and more energetically efficient than the currently established ones, solving the environmental problems associated to the incorrect management of these wastes. For this purpose, the processes are studied at different levels, from the microscopic scale of the involved physical and chemical phenomena, to the design of pilot plants, searching the improvement in the fundamental and methodological knowledge, kinetic modeling, and design and simulation of the process units.

RESEARCH TOPICS

1. Hydrodynamics of the technology of the conical spouted bed reactor, with new configurations and internal devices for controlling gas and solid flow rates, enhancing its versatility for new applications.
2. New gas-solid contact equipment (spouted beds, micro and nanocyclones), for the physical treatment of solids (separation, drying, granulation) up to pilot plant scale, in collaboration with the spin off NOVATTIA.
3. New equipment for the continuous valorization of solid wastes: Biomass (different types) and wastes generated by the consumer society (plastics, sewage sludge and tires). In this bench scale and continuous feeding equipment, thermal transformation processes (pyrolysis, gasification), catalytic ones or their combination are carried out, in a single unit or two in line processes, for the production of hydrogen, syngas or raw materials. This topic investigates the suitability of the conical spouted bed for these processes.
4. Methodological development in the Chemical Reaction Engineering: At the same time of the technologic innovation studies previously commented, the group also contributes to the methodological development of the studied research areas (experimental, theoretical, calculus and design) of the phenomena and equipment. Thus, theoretical contributions are made in: i) the modeling of the spouted bed hydrodynamics, establishing the experimental methodology and the calculus for the characterization and gas and solid flow rates; ii) the kinetic modeling of the reactions (pyrolysis, gasification ...), and; iii) process integration and intensification.

This research topic is developed in collaboration with other universities (European, Canadian, Brazilian, Iranian ...) as it has a worldwide interest. In addition, it also comprises an active the technology transfer to the industry.

For more information: <http://www.ehu.es/cpwv>

Catalytic processes for sustainable refinery

A.T. Aguayo, B. Aramburu, J.M. Arandes, A. Arandia, A. Ateka, M.J. Azkoiti, J. Bilbao, P. Castaño, T. Cordero-Lanzac, M. Díaz, J. Ereña, M. Gamero, A.G. Gayubo, A. Gutiérrez, I. Hita, M. Ibáñez, A. Ibarra, L. Oar-Arteta, A. Ochoa, R. Palos, P. Pérez-Uriarte, A. Remiro, E. Rodríguez, P. Rodríguez-Vega, M. Sánchez-Contador, I. Sierra, J. Valecillos, B. Valle

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KEY WORDS: Catalytic processes, bio-refinery, waste-refinery

INTRODUCTION AND OBJECTIVES

The research lines of the Catalytic Processes and Waste Valorization (CPWV) group deal with: i) the development of new catalytic processes and; ii) the revamping and improvement of those already implemented in refinery. Our efforts are focused on obtaining raw materials and fuels from sources alternative to oil and intensifying its recovery, by means of environmentally friendly routes.

The activities of the research group are framed in two major research areas: 1) Bio-Refinery and; 2) Waste-Refinery, aimed for obtaining results of excellence and social interest, giving response to current challenges regarding energy and sustainability. For this purpose, the processes are studied at different levels, from the microscopic scale of the involved physical and chemical phenomena, to the industrial design and scaling, pursuing the improvement in different fields of knowledge: fundamental and methodological, kinetic modeling, and design and simulation of the process units.

RESEARCH LINES

1. Production of H_2 by catalytic reforming (steam, oxidative and autothermal reforming) of biomass derived compounds (bio-oil, ethanol, dimethyl ether).
2. Upgrading of refinery processes (cracking, hydrogenation and hydrocracking) for the valorization of waste (derived from the pyrolysis of biomass, plastics and tires) and streams of secondary interest (coker naphtha, light cycle oil...).
3. Valorization of CO_2 by the synthesis of DME, designing enhanced bifunctional catalyst (core shell) and reactors (membrane reactors to remove H_2O).
4. Other catalytic processes of energetic and environmental interest. Among these: the production of olefins from paraffins and oxygenates (DME, ethanol) and its mixtures; the production of olefins from methane (via chloromethane) and; fuel production via olefin oligomerization.
5. Catalyst deactivation control, by understanding the mechanisms and pathways (coke deposition, sintering...), tailoring the properties of the catalyst and establishing deactivation kinetics and process strategies.
6. *Methodological development in Chemical Reaction Engineering*. In parallel with the technological innovation studies described previously and according to its academic nature, the group contributes to the methodological development in the different fields of study (experimental, theoretical, calculation and design) of phenomena and equipment. The study objectives are: the techniques of catalyst preparation and characterization; the knowledge of the reaction and deactivation mechanisms; the methods for data analysis and kinetic modeling, and; the design and simulation of catalytic reactors.

For more information: <http://www.ehu.es/cpwv>

Chemical Engineering in Energy and Environment (Energamb)

Ana de Luis, Natalia Villota, Janire Mardaras, Amaia Menéndez, José Maria Lomas, Cristian Ferreiro, Jose Ignacio Lombrana.

KEY WORDS: advanced oxidation, emerging pollutants, microwave drying, fuel cells.

Within the area of Chemical Engineering, the research activity of group, named: *Ingeniería Química en Energía y Medioambiente* (IQE&MA or Energamb), is centered in aspects related to the studies of residual water treatment based on advanced oxidation technologies, oriented either on solving environmental problems of waters or on searching reusability and benefits on certain industrial effluents. One second part of the activity frames in the study of energy production systems through fuel cells and the application of microwave heating processes (dielectric heating). Some details related to the referred research areas are mentioned in the next:

1. In the environmental area. The investigation is centered in the knowledge of the kinetic mechanisms of the reactions of oxidation based on the action of hydroxyl radicals HO^\bullet appearing in all the operations of advanced oxidation. The knowledge is applied to the effective design of oxidation equipment enabling degradation pollutants, based on the use of H_2O_2 and O_3 like oxidants, and their combination with radiation UV, salts of Fe (II) and TiO_2 for the removing of pollutant compounds in waste waters.

Related to the environmental sustainability, in the last years, the group also projects its research activity to the remediation of the environmental impact due the emerging pollutants within collaborative actions with other UPV/EHU research groups in the ecotoxicology area. Currently, studies are developed on the presence of emergings in waste waters, as well as on their effects and remediation, in which private and public organizations like *Consorcio de Aguas Bilbao Bizkaia* are involved. One of our aims is to achieve treatment technologies on the basis of the integration of advanced oxidation processes (using O_2 and H_2O_2) and membrane (extreme and nano-filtration) for a control and safe reusability of the residual effluents.

2. In energy. Microwaves energy as heating form is an important section in which the research of our group is centered. It has been applied successfully to the design of technologies of drying at low temperature, with similar quality and minor cost than those obtained by lyophilization. Many problems like those related to the high heat transmission resistances by thermal gradient are eliminated. The most favorable conditions for the development of drying equipments are studied to obtain greater energy efficiency and quality in the dehydrated products than those by conventional heating. Noteworthy is the drying by microwaves in fluidized bed for the stabilization of microencapsulated probiotic material, greatly applied to the elaboration of functional foods.

On the other hand, the present situation of the technology of fuel cells in relation to the energy crisis and the environmental global problems due to fossil fuels signals the fuel cells of hydrogen PEM - FC like one of the alternatives with greater possibilities. In this field, critical aspects like the catalyst, the polymeric membrane (currently dominated by the perfluorated membranes like Nafion) and the hydrogen source are investigated.

EMAKUME IKERTZAILEAK MUJERES INVESTIGADORAS



Some information about the participation in the 5th Conference on Research of the Faculty of Science and Technology

Ainhoa Alonso¹, Arantxa Casillas¹, Marta Macho¹, Osane Oruetxebarria¹, Esther Rebato¹, M^a Asunción Requero¹, Efraim Reyes¹, Raquel Torralba¹ and Arantxa Urkaregi¹

¹Equality Committee of the Faculty of Science and Technology (UPV/EHU).

KEY WORDS: female, gender equality, main researcher, male, research.

The 6th and 7th April the Fifth Conference on Research of the Faculty of Science and Technology was hold. The Committee of Equality of the Centre decided to analyse the information collected by the organizers about the profile of the Research Groups that develop their investigation in the Faculty. Our aim was to know which the role of the female is in part of our daily work.

The poster only represents the analysis of the groups that have participated in this Conference. Once this aspect has been explained, we have represented six different graphics related to these three different items: the general participation, the profile of the groups and the oral communications.

1. General participation: 46 research groups have taken part in the conference, totally 453 people being female 256 of them.
2. The profile of the groups: from the 46 groups, 27 of them have a man as main research and 19 of them have managed by a woman. Beside, this item has been dealt with the following three aspects.
 - a. The distribution inside the group which main research is a man.
 - b. The distribution inside the group which main research is a woman. In general, there are more women in groups whose main research is a woman than when is a man.
 - c. Taking the big five areas of the Science in our Faculty, i. e., Biology, Chemistry and Chemistry Engineering Geology, Physics and Electronic Engineering, and Mathematics, how are distributed the groups whose main research is a woman among these areas. In this case, there is not a clear distribution.
3. The oral communications: from the whole of the sort talks given, the presentations made by female have doubled the ones made by male.

To conclude, we want to emphasise that this poster does not represent the real situation of the female researcher in the Faculty. This analysis would need a deeper job recollecting information and treatment of that information.

SGIKER



UPV/EHU mapping research infrastructure

Navarro-Vega, J , Echeverria-Machado, I
SGIker
University of the Basque Country
UPV/EHU

KEY WORDS: research facility, infrastructure, research support, technological development.

Advanced Research Facilities, SGIker, created by the University of the Basque Country / Euskal Herriko Unibertsitatea, UPV/EHU, are born with the vocation to respond and provide support for research, being available to the university itself, other Public Institutions and Businesses.

SGIker have front-line technical and human resources, and aims to offer research support at the highest level, with modern equipment and high technology equipment. This infrastructure allows SGIker to respond to a variety of problems in the field of research and technological development.

Their principal purposes are:

1. Accompany research staff and technologist in their professional career, enhancing the strategy of training, internationalization and dissemination of knowledge, in the different areas of science and technology.
2. Advise and support the personnel of the socioeconomic environment, in the design and development of new methodologies and in the execution of tests, with different scope of accreditation and certification.

SUBTITLE

SGIker Units are distributed in three of the historical territories of the Basque Country and in the different science areas,

1. Material & Surfaces.
2. Biomedicine & Biotechnology.
3. Environment.
4. Common services.
5. Technological Support.
6. Area of Historic-Geographic Science.

BESTE IKERGUNE BATZUK OTROS CENTROS DE INVESTIGACIÓN



156

- 1- Low Carbon
 - 2- Natural Environment
 - 3- Health and Climate
 - 4- Climate Policy
-
- The diagram illustrates the interdisciplinary nature of climate change research. It features three overlapping circles at the top: 'Physical Sciences' (red), 'Economics of Climate Change' (green), and 'Policy Sciences' (blue). Below these, a green box labeled 'Mitigation' is connected by an arrow to a green box labeled 'Low Carbon Climate and Environment'. The 'Economics of Climate Change' circle is positioned directly above the 'Mitigation' box, indicating its central role in the process.



BC3 confirmed its leadership position in the World Top Class ranking of Think Tanks in the field of climate change, economics and policy. The research conducted by the professionals at BC3 and the networks of scientific cooperation to which they belong have consolidated the centre as an international benchmark. The ICCG ranking is a clear recognition of the excellent results of the BC3 in this field.

The ICCG (International Center for Climate Change Governance) has recognized BC3 as a leading institution worldwide in the field of climate change economics and policy among the international top class, and ahead of 293 public and private organisations.

BC3 relies on a multidisciplinary team of 42 people: 37 researchers of several countries who have research careers in some of the most prestigious research centres on the specialty, and 5 members for the Administration area.

- Worldwide Networking
- 21 ongoing International Research Projects
- 15 ongoing National Research Projects
- Over 223 indexed publications in WOS

www.bc3research.org / <http://info.bc3research.org/> <https://twitter.com/bc3research>

BASQUE CENTER FOR APPLIED MATHEMATICS (BCAM)



BCAM - Basque Center for Applied Mathematics

Mazarredo 14, Bilbao, Basque Country, Spain
www.bcamath.org

KEY WORDS: BCAM, mathematics, applied mathematics.

BCAM is a **Basque Excellence Research Center (BERC)**, a world-class interdisciplinary research center on Applied Mathematics created in September 2008 and located in Bilbao. BCAM is formed by more than 50 researchers from 20 nationalities and the average age is less than 35 years.

Mission:

- Perform research in the frontiers of mathematics
- Train and attract talented scientists
- Interact with industry and R&D&I agents, promoting Mathematics in the service of society
- Disseminate mathematics and its applications within society
- Become a relevant node in the international mathematics research network

BCAM was awarded as a **Severo Ochoa Excellence Research Center** in 2014. This accreditation recognizes BCAM as one of the best research centers in its area worldwide.

BCAM main research objectives are structured in the following **Scientific Platforms**:

Core in Applied Mathematics

- Fourier Analysis
- Numerical Analysis
- Partial Differential Equations
- Probability and Statistics

Computational Mathematics

- Modelization
- Computer Simulation
- Numerical Stochastics and Montecarlo methods

Application of Mathematics

- Industry, CFD, Electric...
- Health: Hospital, Images,...
- Social: Finances, net
- Other applications

BCAM research is focused on the Basque specialization areas: Big Data

- **Advanced Manufacturing** Predictive maintenance and repair, Sensoring
- **Energy** Smart Metering, Smart Grid/Power Grid
- **Biosciences** Patient monitoring
- **Epidemiological analysis**
- **Claims Fraud detection**

Examples of simulations done by BCAM researchers:

- Numeric simulation of the propagation of cortical spreading depression in the human brain
- Aircraft: slice aligned with the angle of attack showing the tetrahedra of the starting mesh (a) and finest adadptative mesh (b) for $\alpha = 18,5^\circ$
- Streamlines of velocity around a Wells turbine for wave energy conversion

BCAM - Basque Center for Applied Mathematics

Mazarredo 14, Bilbao, Basque Country, Spain
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KEY WORDS: BCAM, mathematics, applied mathematics.

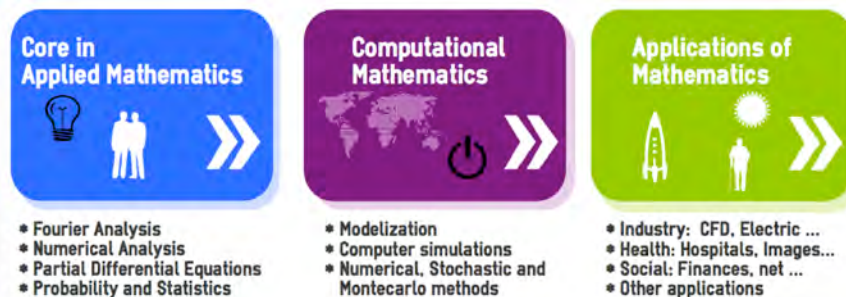
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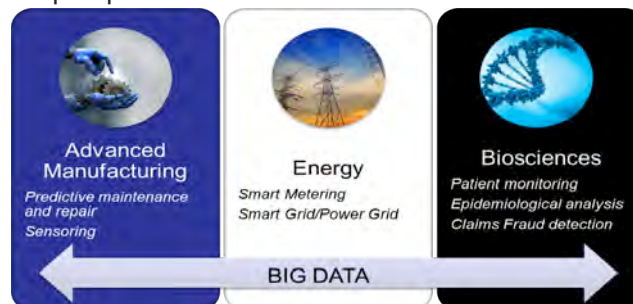
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- Disseminate mathematics and its applications within society
- Become a relevant node in the international mathematics research network

BCAM was awarded as a **Severo Ochoa Excellence Research Center** in 2014. This accreditation recognizes BCAM as one of the best research centers in its area worldwide.

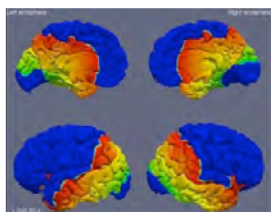
BCAM main research objectives are structured in the following Scientific Platforms:



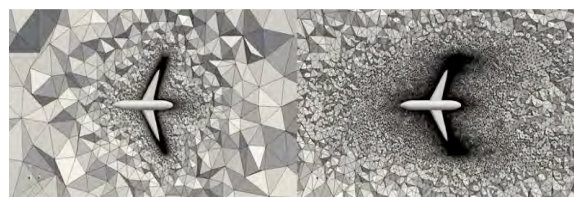
BCAM research is focused on the Basque specialization areas:



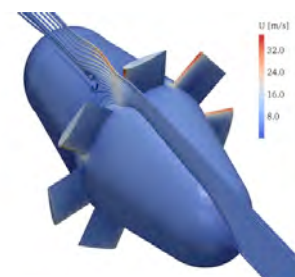
Examples of simulations done by BCAM researchers:



Numeric simulation of the propagation of the cortical spreading depression in the human brain



Aircraft: slice aligned with the angle of attack showing the tetrahedra of the starting mesh (a) and finest adaptive mesh (b) for $\alpha=18.5^\circ$.



Streamlines of velocity around a Wells turbine for wave energy conversion

INSTITUTO BIOFISIKA INSTITUTOA



Instituto Biofisika, a Joint Centre between the University of the Basque Country (UPV/EHU) and the Spanish Research Council (CSIC)

KEY WORDS: Biophysics, biomedicine, biomembrane.

The Instituto Biofisika is a Joint Centre between the University of the Basque Country (UPV/EHU) and the Spanish National Research Centre (CSIC).

Recently we moved to our new location thanks to the help of public Institutions: Basque Government, Biscay County Council, and specially thanks to the firm support of our joint parent institutions, the University of the Basque Country (UPV/EHU) and the Spanish National Research Centre (CSIC), that make possible our sustained activity, even in these difficult times.

The Instituto Biofisika is thriving with devoted scientists, enthusiastic students, technicians and administrators that are our main asset. The Institute is involved in novel advanced projects, both basic and applied, and continues actively pursuing the education of young scientists at the pre- and post-doctoral levels.

The plasma membrane separates the inside of the cell from the outside environment. Also biological membranes are responsible for the internal relationships between different cellular organelles. Both events dictate the healthy functioning of the cell and therefore of the organism. Besides, the membrane is not a static wall and it is home to lipids and many proteins responsible for vital functions that depend on the relationships between these two classes of components. Within these functions it is important to highlight cellular communication, migration and the movement of molecules in and out of the cell. The membrane is also the entrance point for viral and bacterial infection, and other adverse agents. Therefore, comparative studies of the components of the membrane and the relationship between them in healthy and unhealthy states can shed light on important biomedical questions.

Biophysics seeks to answer how biological systems work using an eclectic approach based on the principles of physics and chemistry. For instance, specific molecules involved in a biological process are identified using chemical and biochemical analysis techniques. Likewise, protein molecular structures and interactions are determined using a wide variety of techniques of physics and chemistry. Additionally, the relationship between biological function and molecular structure can be investigated using instruments and techniques of great precision and exquisite physical sensitivity capable of monitoring the properties or movement of groups of atoms. In sum Biophysics explains biological functions in terms of molecular mechanisms with precise physical descriptions of how individual molecules work together as tiny machines to produce specific biological functions.

CIC ENERGIGUNE



Effect of O₂, CO₂ and N₂ gases on clean lithium surfaces: Surface composition and work-function analysis

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KEY WORDS: metallic lithium, anode, batteries

Despite being a really promising anode in terms of capacity, metallic lithium still presents some safety issues for rechargeable batteries. The need of finding a stable Solid Electrolyte Interface (SEI) between the electrolyte and the lithium metal anode which will provide to the battery long term stability at high current densities seems essential^[1]. There have been several studies to find a more stable interface, most of them are focused on the addition of specific additives in the electrolyte^[2].

In this study the SEI layer is formed upon gas exposure in ultra-high vacuum (UHV) of a clean surface of pure lithium, obtaining a non-electrolyte based SEI. Thanks to this method, the lithium will be free from surface impurities, which are supposed to be one of the responsables of short cycling life and low efficiency^[3]. Specifically, this study is focused on the effect that atmospheric gases (O₂, CO₂ and N₂) produce on a clean lithium surface.

CHARACTERIZATION OF THE SURFACE

Photoemission spectroscopy techniques are mainly used to analyze the surfaces: XPS (X-Ray Photoelectron Spectroscopy) which has already been widely used in order to analyze the species that are created on the surface of the treated lithium^[2,4], and UPS (Ultraviolet Photoelectron Spectroscopy) which allow us to determine the work-function (w_f) of the surface. This parameter gives the energy that is required to remove an electron from the surface, on this regard theoretical studies suggest that the created surface after gas exposure is more metallic than lithium itself^[5].

RESULTS

The surface on the lithium has been dosed in UHV condition between 1 and 1000 L, where 1 L equals to a dose at 10⁻⁶ Torr during 1 second. In our studies we saw that the w_f of clean lithium decreases when the surface reacts with O₂ and CO₂ gases: it is easier to withdraw an electron, so the surface becomes “more metallic”. Furthermore, for the same gas dose, the lithium exposed to O₂ gas oxidizes faster than the one reacted with CO₂, being Li₂O the main compound of the oxidized surface. Lithium does not react with N₂ gas at the analyzed gas doses.

The following step is to correlate the w_f values with the electrochemical performance of the cell, and try to find a relationship between both parameters.

[1] Aurbach, D., et al. (1996). *Langmuir*, 12(16), 3991-4007.

[2] Li, W., et al. (2015). *Nature Communications*, 6(May), 1-8.

[3] Harry, K. J., et al. (2014). *Nature Materials*, 13(1), 69-73

[4] Ensling, D., et al. (2008). *Applied Surface Science*, 255, 2517-2523.

[5] Koch, S. L., et al. (2015). *Journal of Power Sources*, 296, 150-161.

Sodium ion battery - A full cell study

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KEY WORDS: sodium, batteries, full cell.

Energy conversion and storage is one of the great challenges of the last decades due to the huge demand increase. Non-renewable sources have a lot of negative aspects, such as the CO₂ emissions and their shortage as a natural resources. Consequently, it is essential to find new efficient, less pollutant and renewable energy sources which are able to replace fossil fuels. For that, it is necessary to develop new systems which store the excess of energy when the demand is low and which are able to supply it at a later stage when the demand is high. That is, efficient, safe, low-cost, and environmentally friendly storage systems, like batteries, are required in response to modern society's needs. Li-ion batteries may have a huge impact on the lithium sources availability and it may not be possible to afford the current demand of lithium compounds in the future. Sodium compounds are cheaper, more abundant and are widely distributed in the Earth's crust; therefore they constitute a possible alternative to Li-ion batteries [1]. Faradion has demonstrated a Na-ion battery with energy density of 140 Wh/kg [2].

RESEARCH DEVELOPMENT

Na-ion batteries are constituted of two sodium insertion materials, cathode and anode, which are separated by a separator and immersed in a liquid electrolyte (sodium salt dissolved in aprotic polar solvents) which is a pure ionic conductor. Na⁺ ions are transported from the cathode through the electrolyte until they reach the anode during the charge with an energy consumption. During the discharge of the battery, the sodium ions return back from the anode to the cathode with an energy release.

Electrochemical characterization of the cathode and the anode, separately, is carried out in order to analyze behavior of each component separately and followed by further study to develop the full-cell with the combination of the electrode materials. In this case, the active material of the cathode is made by a layered oxide transition metal, and the active material of the anode is hard carbon, an amorphous carbon.

The main parameters to optimize in the electrochemical and cycling behavior of a battery are divided by the following steps: electrode slurry preparation, coating, drying, calendaring and the assembly and electrochemical characterization of the battery. Among the different parameters to optimize, it is highlighted the ratio of positive and negative electrode masses, the proportion of the slurry mixture of the compounds which formed the electrodes, the electrode thickness by the process of coating, the charge and discharge cut-off voltages, along with the operating temperature.

RESULTS AND FUTURE WORK

- Full cells with comparable capacity to half cells and ≈3V discharge voltage obtained.
- Experimental Cathode/Anode mass ratio = 1.38 calculated.
- Coulombic efficiency ≈ 100% and capacity retention of 80% obtained after 50 cycles.

In the future, the work will mainly involve the optimization of the mentioned parameters in order to obtain an optimal rechargeable battery.

- Reproducibility studies.
- Find the best processing parameters using coin cells to maximize the anode and cathode performances.
- Reach the capacity values of 1.5mAh by optimizing process parameters.
- Fabrication of pouch cells based on the process parameters optimized at coin cell level.

PLENTZIA MARINE STATION (PIE-UPV/EHU)



Research Centre for Experimental Marine Biology and Biotechnology - Plentzia Marine Station (PiE-UPV/EHU)

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Plentziako Itsas Estazioa, PiE-UPV/EHU. www.ehu.eus/PIE

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KEY WORDS: Ocean Health, Research, Formation, Networking, Transference.

The Research Centre for Experimental Marine Biology and Biotechnology "Plentziako Itsas Estazioa" (PIE; Plentzia Marine Station) is an institution without juridical entity created by the University of the Basque Country (UPV/EHU). The centre is devoted to scientific and technological research; it also carries out teaching activities of specialised education (e.g., postgraduate studies and doctorates), science dissemination; and it might provide technical advice in the field of its expertise in order to transfer to industry and administration those scientific and technological outcomes developed in the areas of interaction between the Ocean and ecosystem and human health and in related disciplines.

SCIENTIFIC BACKGROUND

The promoters of this initiative in the UPV/EHU have been conducting research of excellence in diverse aspects (Cell Biology, Ecology, Analytical Chemistry, etc.) of the interactions between environment (chemical substances and other environmental agents) and living organisms over the last 20 years. Two of these research groups have been recognised as Consolidated Groups "A" and two as Consolidated Groups "B", and are integrated in two Formation and Research Units (UFI11/37 "Ecosystem Health Protection (UFIPSE)" and UFI11/26 "Global Change and Heritage"). In parallel to the research work carried out, big efforts have been addressed to formation (postgraduate and doctorate education, specialization courses, etc.) and dissemination on diverse aspects related to terrestrial and marine ecosystems' health. Thus, two Official Postgraduate Masters with Mention of Quality ("Erasmus Mundus MSc in Marine Environment and Resources" and "Environmental Contamination and Toxicology") are offered as a part of the UPV/EHU Postgraduate Programme. In addition, the Doctoral programmes "Marine Environment and Resources" and "Environmental Contamination and Toxicology" have been recognized with the Mention towards Excellence of the Ministry of Education (2011-to date).

MISSION

- conducts innovative scientific research (basic, strategic and applied) of excellence whose paradigm is the study of the health of the marine ecosystems by means of a bio(techno)logical experimental approach,
- develops (biotechnological) diagnosis tools to analyze and to quantify the health of marine ecosystems,
- explores marine resources that contribute to the protection of the human well-being,
- promotes internationalization by means of networking and attracting junior and senior researchers,
- offers high level postgraduate and doctorate formation and specialization and continuous formation, and offers environmental programs of spreading, awareness and education.

VISION

- leader at European and world-wide scale, recognized by the excellence of its research in the field of ecosystem health science, the quality of the diagnosis tools of developed and applied to assess ocean health, and its contribution to the exploration of marine resources with applications in biomedicine;
- of reference for international institutions and networks, and for talented senior and junior (e.g., doctoral candidates) researchers; and
- recognized within the European Higher Education Area as an excellence center as regards postgraduate, doctoral and of specialist (LLL) education, of science dissemination and environmental awareness.

STRATEGIC AIMS

- To promote and to sustain educational programmes in the field of environmental sciences and education as well as research activity in the area of Experimental Marine Biology and Biotechnology.
- To contribute to postgraduate education and doctorate formation in the context of the European Higher Education Area in aspects related to the environment, and more particularly to the marine environment.
- To develop open activities for science dissemination and specific activities addressed to form specialists and technologists and to achieve Long-Life Learning.

* Deputy director; ** Director; *** Responsible of Experimental Aquaria

POSTER SARITUA PÓSTER GANADOR



IMaCris/MaKrisi Research Team

Development of advanced materials for the generation, storage and liberation of energy

Maribel Arriortua, M. Karmele Urriaga, José L. Pizarro, Gotzone Barandika, Begoña Bazán, Karmele Vidal, Edurne Serrano, Roberto Fernández, Arkaitz Fidalgo, Aroa Morán, Francisco LLano, Eder Amayuelas, Laura Bravo, Aritza Wain e Iñigo Pérez

Mineralogy and Petrology Department. Science and Technology Faculty. University of the Basque Country (UPV/EHU), Sarriena s/n, 48940 Leioa, Bizkaia maribel.arriortua@ehu.es, <http://www.ehu.es/es/web/imacris-makrisi/home>

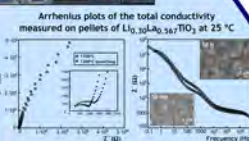
Batteries

Rechargeable

New Laminar Vanadium Cathodes



Solid Electrolytes
Rare Earth Lithium Titanates

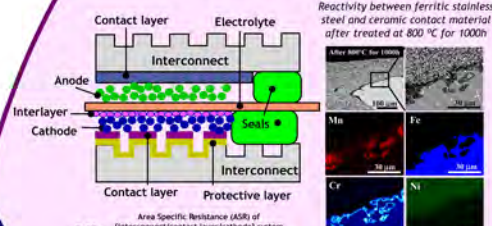


Primary

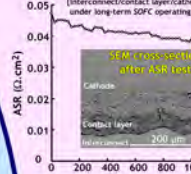
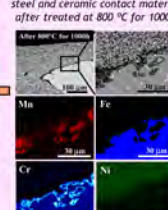
Cathodes based on Silver Nanostructured Hydrogels



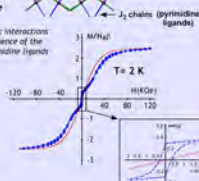
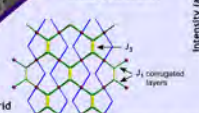
SOFC cells



Reactivity between ferritic stainless steel and ceramic contact material after treated at 800 °C for 1000h



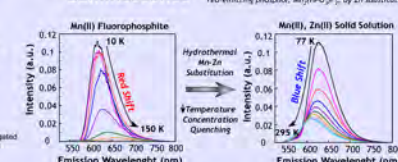
Magnetism



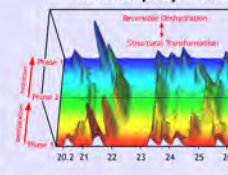
Physical Properties

Luminescence

Enhancement of the luminescent properties of a new red-emitting phosphor, $\text{Mn}(\text{II})\text{PO}_4$, by Zn substitution

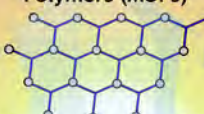


Thermal properties

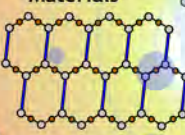


Materials Design

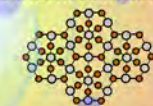
Coordination Polymers (MOFs)



Hybrid Materials



Inorganic Condensed Materials

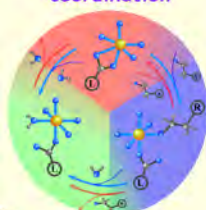


Zeotypes



Sensors

Changing the metal coordination

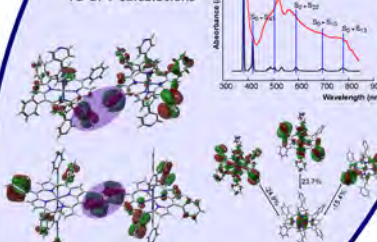


Coordination polymer as chemical sensor
Reversible adsorption of water, ethanol and methanol



DFT Calculations

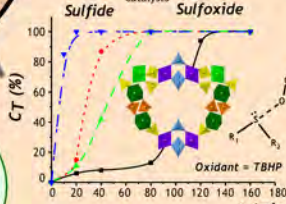
Analysing structural features with DFT and TD-DFT calculations



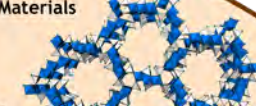
Theoretical Calculations

Catalysis

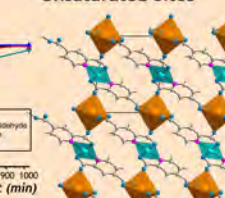
Sulfide catalysts



Porous Materials



MOF with Coordinatively Unsaturated Sites



Catalytic studies with metalloporphyrins have shown are active for acetylation and oxidation of alcohols and amines

Porphyrins found in nature are capable of mimic biological functions

Porphyrins

Collaborations

- School of Chemistry, University of Birmingham.
- Department of Chemical Engineering and Biotechnology, University of Cambridge.
- Laboratoire MADIREL, Aix Marseille Université.
- Department of Chemistry, University of Saint Andrews.
- Ecole Polytechnique Fédérale de Lausanne (Suiza).
- Departamento de Ciencias, Pontificia Universidad Católica del Perú.
- Instituto de Química y de la Materia Condensada, Universidad de Burdeos (Francia)
- Departamento de Ciencias de la Tierra y Física de la Materia Condensada, CITIMAC, Universidad de Cantabria.
- Instituto de Ciencia de Materiales, CSIC, Universidad de Barcelona.
- Departamento de Química Inorgánica, Universidad de La Laguna.
- Instituto de Ciencia de Materiales, ICMM-CSIC, Universidad de Madrid.
- Instituto de Ciencia de Materiales de Aragón, ICMA-CSIC, Universidad de Zaragoza.

Latest Publications

- CrystEngComm, 2016, 18, 1709-1712.
- Int. J. Hydrogen Energy, 2016, DOI: 10.1016/j.ijhydene.2016.02.088
- Eur. J. Inorg. Chem., 2015, 2015, 4699-4707, Solid State Ionics, 2015, 269, 24-29.
- J. Mater. Chem. A, 2015, 3, 19996-20012, CrystEngComm, 2015, 17, 6346-6354.
- J. Solid State Chem., 2015, 230, 191-198, Dalton Trans., 2015, 44, 213-222.
- Int. J. Hydrogen Energy, 2015, 40, 8407-8418, Molecules, 2015, 20, 6683-6699.
- CrystEngComm, 2015, 17, 3297-3304, Polyhedron, 2015, 92, 117-123.
- Int. J. Hydrogen Energy, 2015, 40, 4804-4818, J. Power Sources, 2015, 280, 505.
- "Alcohol and water sensor compounds, detection method and device", PCT Int. Appl. 2013, WO 2013057350 A1 20130425.

Patents

Funding

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- Ministerio de Economía y Competitividad (MEC) (MAT2013-42092-R).
- Unidad de Formación e Investigación de la UPV/EHU (UFI11/15).

The personnel, in training and contracted, are linked to the Ministerio de Economía y Competitividad, to the Departamento de Educación, Política Lingüística y Cultura del Gobierno Vasco, UPV/EHU and to the BCMaterials by grants and pre- and post-doctoral contracts.

